

| | | |
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| <u>NEWS 1</u> | Web Page URLs for STN Seminar Schedule - N. America | |
| <u>NEWS 2</u> | "Ask CAS" for self-help around the clock | |
| <u>NEWS 3</u> | May 10 | PROUSDDR now available on STN |
| <u>NEWS 4</u> | May 19 | PROUSDDR: One FREE connect hour, per account, in both May and June 2004 |
| <u>NEWS 5</u> | May 12 | EXTEND option available in structure searching |
| <u>NEWS 6</u> | May 12 | Polymer links for the POLYLINK command completed in REGISTRY |
| <u>NEWS 7</u> | May 17 | FRFULL now available on STN |
| <u>NEWS 8</u> | May 27 | New UPM (Update Code Maximum) field for more efficient patent SDIs in CAplus |
| <u>NEWS 9</u> | May 27 | CAplus super roles and document types searchable in REGISTRY |
| <u>NEWS 10</u> | May 27 | Explore APOLLIT with free connect time in June 2004 |
| <u>NEWS 11</u> | Jun 22 | STN Patent Forums to be held July 19-22, 2004 |

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 21 JUN 2004 HIGHEST RN 697224-75-2
DICTIONARY FILE UPDATES: 21 JUN 2004 HIGHEST RN 697224-75-2

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>
 L1 STRUCTURE UPLOADED

=> d 11
 L1 HAS NO ANSWERS
 L1 STR

=> s 11
 SAMPLE SEARCH INITIATED 19:21:50 FILE 'REGISTRY'
 SAMPLE SCREEN SEARCH COMPLETED - 8863 TO ITERATE

11.3% PROCESSED 1000 ITERATIONS 4 ANSWERS
 INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
 SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
 BATCH **COMPLETE**
 PROJECTED ITERATIONS: 171619 TO 182901
 PROJECTED ANSWERS: 352 TO 1066

L2 4 SEA SSS SAM L1

=> s 11 full
 THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS
 DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
 FULL SEARCH INITIATED 19:21:54 FILE 'REGISTRY'
 FULL SCREEN SEARCH COMPLETED - 175967 TO ITERATE

100.0% PROCESSED 175967 ITERATIONS 579 ANSWERS
 SEARCH TIME: 00.00.07

L3 579 SEA SSS FUL L1

=> file hcaplus
 COST IN U.S. DOLLARS SINCE FILE TOTAL
 ENTRY SESSION
 FULL ESTIMATED COST 155.42 155.63

FILE 'HCAPLUS' ENTERED AT 19:22:04 ON 22 JUN 2004
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FILE COVERS 1907 - 22 Jun 2004 VOL 140 ISS 26
 FILE LAST UPDATED: 21 Jun 2004 (20040621/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 13/thu
 108 L3
 600602 THU/RL
 L4 39 L3/THU
 (L3 (L) THU/RL)

=> s 14 and arthritis?
 32853 ARTHRITIS?
 L5 6 L4 AND ARTHRITIS?

=> s 15 and faull, a?/au
 34 FAULL, A?/AU
 L6 1 L5 AND FAULL, A?/AU

=> d 16, ibib abs fhitstr, 1

L6 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Citing
 Text References

ACCESSION NUMBER: 1999:126819 HCAPLUS
 DOCUMENT NUMBER: 130:182354
 TITLE: Preparation of substituted indoles for treatment of a disease or condition mediated by monocyte chemoattractant protein-1 (MCP-1)
 INVENTOR(S): Barker, Andrew John; Kettle, Jason Grant; **Faull, Alan Wellington**
 PATENT ASSIGNEE(S): Zeneca Limited, UK
 SOURCE: PCT Int. Appl., 64 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

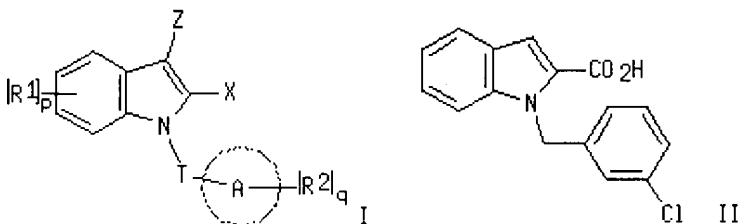
| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------|--|----------|-----------------|----------|
| WO 9907351 | A2 | 19990218 | WO 1998-GB2341 | 19980804 |
| WO 9907351 | A3 | 19990514 | | |
| W: | AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | |
| RW: | GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | |
| AU 9886381 | A1 | 19990301 | AU 1998-86381 | 19980804 |
| AU 745907 | B2 | 20020411 | | |
| EP 1003504 | A2 | 20000531 | EP 1998-937659 | 19980804 |
| EP 1003504 | B1 | 20030702 | | |
| R: | AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI | | | |

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|-------------------------------|----|----------|--------------------------|-------------|
| <u>BR 9811818</u> | A | 20000815 | <u>BR 1998-11818</u> | 19980804 |
| <u>TR 200000289</u> | T2 | 20000821 | <u>TR 2000-200000289</u> | 19980804 |
| <u>JP 2001513494</u> | T2 | 20010904 | <u>JP 2000-506944</u> | 19980804 |
| <u>RU 2217142</u> | C2 | 20031127 | <u>RU 2000-105901</u> | 19980804 |
| <u>PT 1003504</u> | T | 20031128 | <u>PT 1998-937659</u> | 19980804 |
| <u>ZA 9807090</u> | A | 19990208 | <u>ZA 1998-7090</u> | 19980806 |
| <u>HR 2000000061</u> | A1 | 20001231 | <u>HR 2000-61</u> | 20000203 |
| <u>US 6441004</u> <i>—110</i> | B1 | 20020827 | <u>US 2000-485061</u> | 20000203 |
| <u>NO 2000000573</u> | A | 20000204 | <u>NO 2000-573</u> | 20000204 |
| <u>HK 1027979</u> | A1 | 20031031 | <u>HK 2000-107435</u> | 20001121 |
| <u>US 2003119830</u> | A1 | 20030626 | <u>US 2002-194969</u> | 20020715 |
| <u>RITY APPLN. INFO.:</u> | | | <u>GB 1997-16657</u> | A 19970807 |
| | | | <u>WO 1998-GB2341</u> | W 19980804 |
| | | | <u>US 2000-485061</u> | A1 20000203 |

OTHER SOURCE(S)

OTHER SOURCE(S) : MARPAT 130:182354

GI



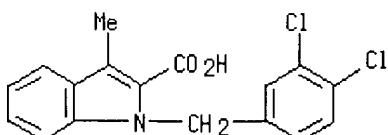
AB The title compds. [I; R1 = CF₃, alkyl, halo, etc.; p = 0-4; T = (CHR₄)_m (wherein R₄ = H, alkyl; m = 1-3); X = CO₂R₄, SO₃H, CN, etc.; A = Ph, naphthyl, furyl, etc.; R₂ = CF₃, alkyl, halo, etc.; q = 0-4; Z = H, halo, Me, etc.] and their pharmaceutically acceptable salts or in vivo hydrolysable esters, useful in the treatment of a disease or condition mediated by monocyte chemoattractant protein-1 (MCP-1) such as rheumatoid **arthritis**, asthma, atherosclerosis, psoriasis, inflammatory bowel disease and stroke, were prep'd. and formulated. Thus, hydrolysis of Et N-(3-chlorobenzyl)indole-2-carboxylate with 2N NaOH in THF/MeOH afforded 82% II. The tested compds. I showed generally IC₅₀ of < 50 μM in the hMCP-1 receptor binding assay.

IT 220678-49-9P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of substituted indoles for treatment of a disease or condition mediated by monocyte chemoattractant protein-1 (MCP-1))

RN 220678-49-9 HCAPLUS

CN 1H-Indole-2-carboxylic acid, 1-[(3,4-dichlorophenyl)methyl]-3-methyl- (9CI) (CA INDEX NAME)



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(FILE 'HOME' ENTERED AT 19:21:10 ON 22 JUN 2004)

FILE 'REGISTRY' ENTERED AT 19:21:16 ON 22 JUN 2004

L1 STRUCTURE uploaded

L2 4 S L1

L3 579 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 19:22:04 ON 22 JUN 2004

L4 39 S L3/THU

L5 6 S L4 AND ARTHRITIS?

L6 1 S L5 AND FAULL, A?/AU

=> s 15 not 16

L7 5 L5 NOT L6

=> d 17, ibib abs fhitstr, 1-5

L7 ANSWER 1 OF 5 HCAPLUS COPYRIGHT 2004 ACS on STN

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|------|------------|
| Full | Citing |
| Text | References |

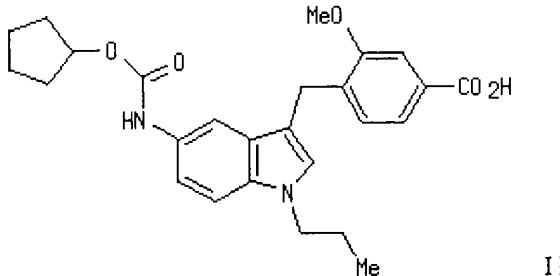
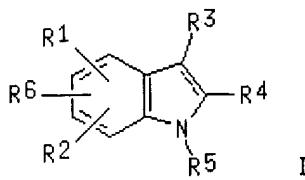
ACCESSION NUMBER: 2003:1275 HCAPLUS
 DOCUMENT NUMBER: 138:55866
 TITLE: Preparation of indole derivatives as phospholipase
 enzyme inhibitors for treatment of inflammatory
 conditions
 INVENTOR(S): Seehra, Jasbir S.; McKew, John C.; Lovering, Frank;
 Bemis, Jean E.; Xiang, Yibin; Chen, Lihren; Knopf,
 John L.
 PATENT ASSIGNEE(S): Genetics Institute, LLC, USA
 SOURCE: U.S., 57 pp., Cont.-in-part of U. S. Ser. No. 256,062,
 abandoned.
 CODEN: USXXAM
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|------|----------|-----------------|-------------|
| US 6500853 | B1 | 20021231 | US 2000-686616 | 20001011 |
| PRIORITY APPLN. INFO.: | | | US 1998-113674P | P 19980228 |
| | | | US 1999-256062 | B2 19990224 |

OTHER SOURCE(S): MARPAT 138:55866

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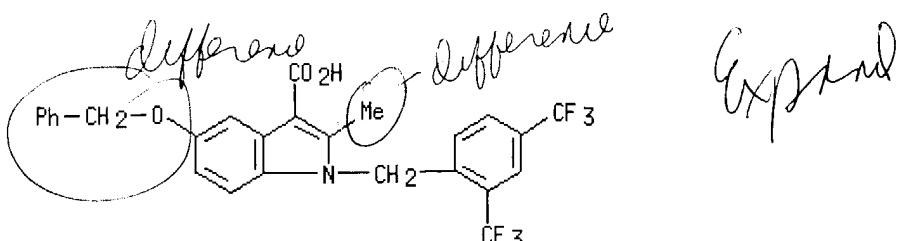


AB Title compds. I [wherein R1 and R6 = independently H, halo, CF₃, alkyl, alkylthio, alkoxy, CN, NO₂, NH₂, Ph, OPh, SPh, CH₂Ph, OCH₂Ph, SCH₂Ph, or (un)substituted amido, carbamido, sulfonyl, etc.; R2 = H, halo, CF₃, OH, alkyl, alkoxy, CHO, CN, NO₂, (un)substituted amino, or alkylsulfonyl; R3 = CO₂H, OPO₃H₂, SO₃H, etc.; R4 = H, CF₃, alkyl, alkoxy, (alkyl)cycloalkyl, CHO, halo, etc.; R5 = alkyl, alkoxy, (alkyl)cycloalkyl, etc.; and pharmaceutically acceptable salts thereof] were prep'd. as phospholipase enzyme inhibitors. For example, 5-nitroindole was C3-alkylated (55%) with Me 4-(bromomethyl)-3-methoxybenzoate in dioxane, N-alkylated (57%) with 1-iodopropane in a soln. of THF and NaH, and converted to the amine (80%) by hydrogenation using Pt/C. The amine was converted to the carbamate (39%) by addn. of cyclopentyl chloroformate in CH₂Cl₂ and 4-methylmorpholine, and the resultant ester was hydrolyzed to yield II (71%). The latter inhibited cytosolic phospholipase A2 (cPLA2) by 50% at a concn. of 170 μM in a coumarin assay and reduced footpad vol. by 16.61% at a dose of 5 mg/Kg IV in a carrageenan-induced footpad edema test on rats. Thus, I are useful for treatment of inflammatory conditions, such as **arthritis**, inflammatory bowel disease, and asthma (no data).

IT 241497-82-5P, 1H-Indole-3-carboxylic acid, 1-[[2,4-bis(trifluoromethyl)phenyl]methyl]-2-methyl-5-(phenylmethoxy)-
RL: PAC (Pharmacological activity); RCT (Reactant); THU (Therapeutic use); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(phospholipase inhibitor; prep'n. of indole derivs. as phospholipase enzyme inhibitors for treatment of inflammatory conditions)

RN 241497-82-5 HCAPLUS

CN 1H-Indole-3-carboxylic acid, 1-[[2,4-bis(trifluoromethyl)phenyl]methyl]-2-methyl-5-(phenylmethoxy)- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

83

THERE ARE 83 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

Full Text Citing References

ACCESSION NUMBER: 2002:964145 HCAPLUS
 DOCUMENT NUMBER: 138:19491
 TITLE: A method for treating inflammatory diseases by
 administering a PPAR- δ agonist
 INVENTOR(S): Forrest, Michael J.; Berger, Joel P.; Moller, David
 E.; Wright, Samuel
 PATENT ASSIGNEE(S): Merck & Co., Inc., USA
 SOURCE: PCT Int. Appl., 33 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|-----------------|------------|
| WO 2002100351 | A2 | 20021219 | WO 2002-US20974 | 20020607 |
| WO 2002100351 | A3 | 20030501 | | |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |
| EP 1399151 | A2 | 20040324 | EP 2002-746824 | 20020607 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR | | | | |
| <u>PRIORITY APPLN. INFO.:</u> | | | US 2001-297356P | P 20010611 |
| | | | WO 2002-US20974 | W 20020607 |

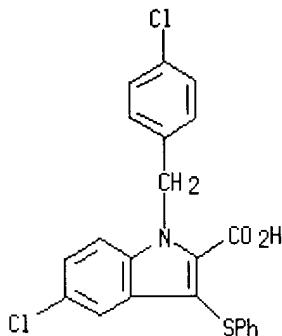
AB A method for treating, controlling, preventing or reducing the risk of contracting an inflammatory disease or condition in a mammalian patient, comprises (1) selecting a patient in need thereof, and (2) treating the patient with a therapeutically effective amt. of a compn. comprising a PPAR- δ agonist. Inflammatory diseases that may be treated by this method include but are not limited to rheumatoid **arthritis**, juvenile rheumatoid **arthritis**, systemic lupus erythematosus, osteoarthritis, degenerative joint disease, one or more connective tissue diseases, ankylosing spondylitis, and bursitis.

IT 118414-59-8

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
 (PPAR- δ agonist for treating inflammatory disease, and use with other agents)

RN 118414-59-8 HCAPLUS

CN 1H-Indole-2-carboxylic acid, 5-chloro-1-[(4-chlorophenyl)methyl]-3-(phenylthio)- (9CI) (CA INDEX NAME)



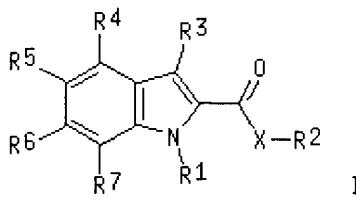
L7 ANSWER 3 OF 5 HCAPLUS COPYRIGHT 2004 ACS on STN

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|-----------|-------------------|
| Full Text | Citing References |
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ACCESSION NUMBER: 2002:293620 HCAPLUS
 DOCUMENT NUMBER: 136:309846
 TITLE: Preparation of substituted indoles as PPAR- γ binding agents
 INVENTOR(S): Stolle, Andreas; Dumas, Jacques P.; Carley, William; Coish, Phillip D. G.; Magnuson, Steven R.; Wang, Yamin; Nagarathnam, Dhanapalan; Lowe, Derek B.; Su, Ning; Bullock, William H.; Campbell, Ann-Marie; Qi, Ning; Baryza, Jeremy L.; Cook, James H.
 PATENT ASSIGNEE(S): Bayer Corporation, USA
 SOURCE: PCT Int. Appl., 233 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|-----------------|------------|
| WO 2002030895 | A1 | 20020418 | WO 2001-US42644 | 20011009 |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |
| AU 2002011901 | A5 | 20020422 | AU 2002-11901 | 20011009 |
| US 2003087902 | A1 | 20030508 | US 2001-974319 | 20011009 |
| EP 1341761 | A1 | 20030910 | EP 2001-979996 | 20011009 |
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| NO 2003001619 | A | 20030602 | NO 2003-1619 | 20030409 |
| <u>PRIORITY APPLN. INFO.:</u> | | | US 2000-239195P | P 20001010 |
| | | | US 2000-243665P | P 20001027 |
| | | | WO 2001-US42644 | W 20011009 |

OTHER SOURCE(S): MARPAT 136:309846
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AB The title compds. [I; R1 = R8R9; R8 = alkyl, alkenyl, alkynyl, etc.; R9 = (un)substituted Ph, cycloalkyl, heterocycloalkyl, etc.; X = (un)substituted NH, S, O; R2 = H, alkyl, halo, alkyl, etc.; R3 = R12R13; R12 = alkyl, alkenyl, alkynyl, CO; R13 = (un)substituted cycloalkyl, cycloalkenyl, heterocycloalkyl, etc.; R4-R7 = H, OH, etc.], useful in treating or preventing PPAR- γ mediated diseases or conditions, such as osteopenia, osteoporosis, cancer, diabetes and atherosclerosis, were prep'd. Thus, hydrolysis of Et 3-(cyclopropylidenemethyl)-1-[3-(trifluoromethyl)benzyl]-1H-indole-2-carboxylate (prepn. given) with NaOH in H₂O/THF afforded 57% I [R1 = 3-F₃CC₆H₄CH₂; X = O; R2 = H; R3 = cyclopropylidenemethyl; R4-R7 = H] which showed IC₅₀ of 100 pM and 9.99 nM against PPAR- γ binding.

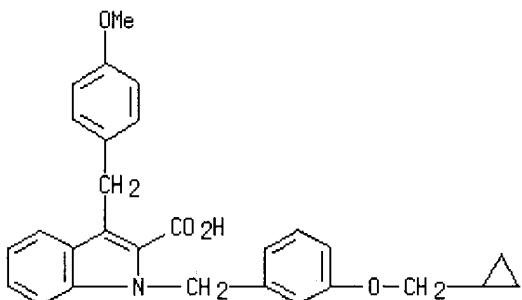
IT 412004-67-2P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of substituted indoles as PPAR- γ binding agents)

RN 412004-67-2 HCAPLUS

CN 1H-Indole-2-carboxylic acid, 1-[[3-(cyclopropylmethoxy)phenyl]methyl]-3-[(4-methoxyphenyl)methyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

10

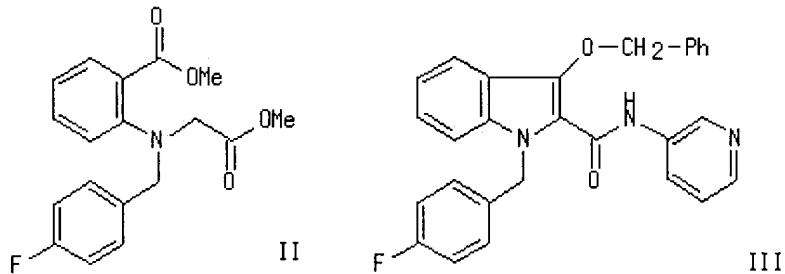
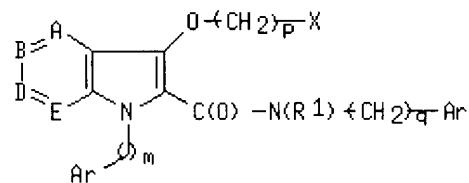
THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 4 OF 5 HCAPLUS COPYRIGHT 2004 ACS on STN

| | |
|-----------|-------------------|
| Full Text | Citing References |
|-----------|-------------------|

ACCESSION NUMBER: 2001:661388 HCAPLUS
 DOCUMENT NUMBER: 135:226878
 TITLE: Synthesis of N-benzyl-indolyl(benzyloxy)amido derivatives as PDE-IV inhibitors
 INVENTOR(S): Labelle, Marc; Sturino, Claudio; Lachance, Nicolas; MacDonald, Dwight
 PATENT ASSIGNEE(S): Merck Frosst Canada & Co., Can.
 SOURCE: PCT Int. Appl., 75 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|------|--|-----------------|------------|
| WO 2001064639 | A2 | 20010907 | WO 2001-CA270 | 20010302 |
| WO 2001064639 | A3 | 20020228 | | |
| | W: | AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | |
| | RW: | GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | |
| US 2002068756 | A1 | 20020606 | US 2001-797083 | 20010301 |
| US 6416965 | B2 | 20020820 | | |
| EP 1263728 | A2 | 20021211 | EP 2001-913422 | 20010302 |
| | R: | AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR | | |
| JP 2003525273 | T2 | 20030826 | JP 2001-563482 | 20010302 |
| PRIORITY APPLN. INFO.: | | | US 2000-186571P | P 20000302 |
| | | | WO 2001-CA270 | W 20010302 |
| OTHER SOURCE(S): | | MARPAT 135:226878 | | |
| GI | | | | |



AB Title compds. I [A, B, D, E = N or CR₂ and the others = CR₂; q = 0 - 1; p, m = 0 - 2; R₁ = H, (hydroxy)alkyl; R₂ = H, halo, (halo)alkyl, hydroxyalkyl, CN, arom. or nonarom. ring system contg. 1 - 4 heteroatoms selected from O, S, N, alkoxy, oxyamide, etc.; X = cycloalkyl or Ar; Ar = (un)substituted (Ph, thieryl, thiazolyl, pyridyl, oxazolyl, tetrazolyl, pyrimidinyl, pyrazinyl and pyridazinyl)] were prep'd. Over 150 compds. were disclosed. For instance, Me 2-aminobenzoate was alkylated with 4-fluorobenzyl bromide (K₂CO₃, MEK, reflux, 8 h.). The resulting ester was saponified (NaOH, MeOHaq reflux, 2 h.), N-alkylated with Me bromoacetate (K₂CO₃, MeOHaq, reflux, 18 h.) and treated with CH₂N₂ to afford II. Diester II was cyclized (NaOMe, MeOH, reflux, 30 min.), O-alkylated with benzyl bromide (K₂CO₃, MEK, reflux, 2 h.), saponified (NaOH, EtOHaq, 90°C, 40 min.) and finally coupled to 3-aminopyridine (SOCl₂, i-Pr₂NEt, room temp., 3 h.) to yield III. I are PDE-IV inhibitors (no

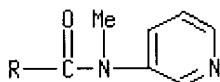
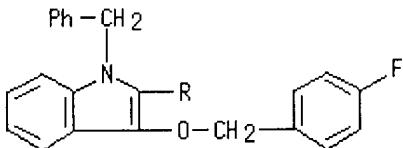
data) useful for treating, e.g., inflammation, muscle spasm, chronic bronchitis, etc.

IT 359001-30-2P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (drug; synthesis of N-benzyl-indolyl(benzyloxy)amido derivs. as PDE-IV inhibitors)

RN 359001-30-2 HCAPLUS

CN 1H-Indole-2-carboxamide, 3-[(4-fluorophenyl)methoxy]-N-methyl-1-(phenylmethyl)-N-3-pyridinyl- (9CI) (CA INDEX NAME)



L7 ANSWER 5 OF 5 HCAPLUS COPYRIGHT 2004 ACS on STN

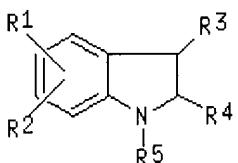
Full Citing
 Text References

ACCESSION NUMBER: 1999:566026 HCAPLUS
 DOCUMENT NUMBER: 131:199619
 TITLE: Preparation of indole derivatives as phospholipase enzyme inhibitors
 INVENTOR(S): Seehra, Jasbir S.; Mckew, John C.; Lovering, Frank; Bemis, Jean E.; Xiang, Yibin; Chen, Lihren; Knopf, John L.
 PATENT ASSIGNEE(S): Genetics Institute, Inc., USA
 SOURCE: PCT Int. Appl., 182 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

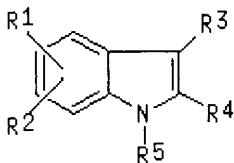
| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---------------------|--|----------|--------------------------|----------|
| <u>WO 9943654</u> | A2 | 19990902 | <u>WO 1999-US3898</u> | 19990224 |
| <u>WO 9943654</u> | A3 | 19991028 | | |
| W: | AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | |
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| <u>CA 2322162</u> | AA | 19990902 | <u>CA 1999-2322162</u> | 19990224 |
| <u>AU 9927825</u> | A1 | 19990915 | <u>AU 1999-27825</u> | 19990224 |
| <u>AU 765427</u> | B2 | 20030918 | | |
| <u>BR 9908275</u> | A | 20001024 | <u>BR 1999-8275</u> | 19990224 |
| <u>TR 200002447</u> | T2 | 20001121 | <u>TR 2000-200002447</u> | 19990224 |

| | | | | |
|---|----|----------|----------------|------------|
| EP 1062205 | A2 | 20001227 | EP 1999-908378 | 19990224 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI | | | | |
| JP 2002504541 | T2 | 20020212 | JP 2000-533412 | 19990224 |
| EE 200000488 | A | 20020215 | EE 2000-488 | 19990224 |
| NO 2000004219 | A | 20001023 | NO 2000-4219 | 20000823 |
| HR 2000000551 | A1 | 20010430 | HR 2000-551 | 20000824 |
| BG 104779 | A | 20011031 | BG 2000-104779 | 20000919 |
| PRIORITY APPLN. INFO.: | | | US 1998-30592 | A 19980225 |
| | | | WO 1999-US3898 | W 19990224 |

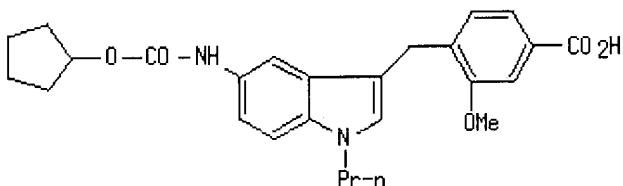
OTHER SOURCE(S): MARPAT 131:199619
GI



I



II



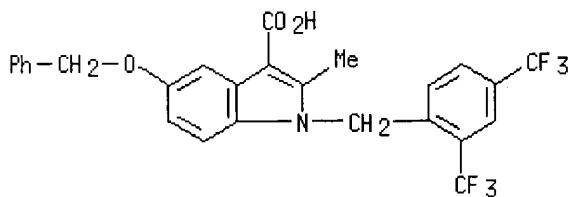
III

AB Indole derivs. (I) and (II) [where R1 = H, halogen, CF3, C1-10 alkyl, S-C1-10 alkyl, C1-10 alkoxy, CN, NO2, NH2, Ph, OPh, SPh, CH2Ph, OCH2Ph, SCH2Ph, or (un)substituted amido, carbamido, sulfonyl, etc.; R2 = H, halogen, CF3, OH, C1-10 alkyl, C1-10 alkoxy, CHO, CN, NO2, (un)substituted amino, SO2-C1-6 alkyl; R3 = (un)substituted carboxylic acid, OPO3H2, SO3H, etc.; R4 = H, CF3, C1-6 alkyl, C1-6 alkoxy, (C1-6 alkyl)cycloalkyl, CHO, halogen, etc.; R5 = C1-6 alkyl, C1-6 alkoxy, (C1-6 alkyl)cycloalkyl, etc.] and pharmaceutically acceptable salts thereof, were prep'd. by several methods. Thus, 5-nitroindole was C3-alkylated with Me 4-(bromomethyl)-3-methoxybenzoate in dioxane, N-alkylated with 1-iodopropane in a soln. of THF and NaH, and converted to the amine by hydrogenation over Pt/C. The amine was converted to the carbamate by addn. of cyclopentyl chloroformate in CH2Cl2 and 4-methylmorpholine and the resultant ester hydrolyzed to yield 4-[(5-[(cyclopentyloxy)carbonyl]amino)-1-propyl-1H-indol-3-yl)methyl]-3-methoxybenzoic acid (III). The title compds. are useful as phospholipase enzyme inhibitors, esp. cytosolic phospholipase A2 (cPLA2), for treatment of inflammatory conditions, particularly where inhibition of prodn. of prostaglandins, leukotrienes, and PAF are all desired. Over one hundred compds. of the invention were tested for cPLA2 inhibiting activity in the Coumarine assay and rat carrageenan-induced footpad edema test. Compds. exhibited 7% to 98% inhibition at concns. of 0.125 μ M to 400 μ M in the Coumarine assay and -7.16% to 34.52% inhibition at concns. of 2 μ M to 20 μ M in the footpad edema test.

IT 241497-82-5P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); **THU (Therapeutic use)**; **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses) (prepn. of indole derivs. as phospholipase enzyme inhibitors for treatment of inflammatory conditions)

RN 241497-82-5 HCAPLUS
 CN 1H-Indole-3-carboxylic acid, 1-[[2,4-bis(trifluoromethyl)phenyl]methyl]-2-methyl-5-(phenylmethoxy)- (9CI) (CA INDEX NAME)



=> d his

(FILE 'HOME' ENTERED AT 19:21:10 ON 22 JUN 2004)

FILE 'REGISTRY' ENTERED AT 19:21:16 ON 22 JUN 2004

L1 STRUCTURE uploaded
 L2 4 S L1
 L3 579 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 19:22:04 ON 22 JUN 2004

L4 39 S L3/THU
 L5 6 S L4 AND ARTHRITIS?
 L6 1 S L5 AND FAULL, A?/AU
 L7 5 S L5 NOT L6

=> s 14 not 15
 L8 33 L4 NOT L5

=> s 18 and glomerular?
 25328 GLOMERULAR?
 L9 0 L8 AND GLOMERULAR?

=> s 18 and lung () fibrosis?
 155142 LUNG
 39674 LUNGS
 168664 LUNG
 (LUNG OR LUNGS)
 25885 FIBROSIS?
 1388 LUNG (W) FIBROSIS?
 L10 0 L8 AND LUNG (W) FIBROSIS?

=> s 18 and restenosis?
 5619 RESTENOSIS?
 L11 2 L8 AND RESTENOSIS?

=> s 111 and faull, a?/au
 34 FAULL, A?/AU
 L12 0 L11 AND FAULL, A?/AU

=> s 111 and kettle, j?/au
 39 KETTLE, J?/AU
 L13 0 L11 AND KETTLE, J?/AU

=> d 111, ibib abs fhitstr, 1-2

L11 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2004 ACS on STN

| | |
|-----------|-------------------|
| Full Text | Citing References |
|-----------|-------------------|

ACCESSION NUMBER: 2001:319722 HCPLUS
 DOCUMENT NUMBER: 134:320871
 TITLE: Pharmaceuticals for treating obesity containing
 antagonists and partial agonists of PPAR- γ
 INVENTOR(S): Berger, Joel P.; Doepper, Thomas W.; Leibowitz, Mark;
 Moller, David E.; Mosley, Ralph T.; Tolman, Richard
 L.; Ventre, John; Zhang, Bei B.; Zhou, Gaochao
 MERCK & CO., Inc., USA
 PATENT ASSIGNEE(S): PCT Int. Appl., 49 pp.
 SOURCE: CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|-------------------------------|--|----------|-----------------|-------------|
| WO 2001030343 | A1 | 20010503 | WO 2000-US28924 | 20001019 |
| W: | AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | |
| RW: | GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | |
| EP 1284728 | A1 | 20030226 | EP 2000-973670 | 20001019 |
| R: | AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL | | | |
| JP 2003525217 | T2 | 20030826 | JP 2001-532763 | 20001019 |
| US 2003032581 | A1 | 20030213 | US 2002-241106 | 20020911 |
| <u>PRIORITY APPLN. INFO.:</u> | | | US 1999-161225P | P 19991022 |
| | | W0 | US 2000-691955 | A3 20001019 |
| | | | WO 2000-US28924 | W 20001019 |

OTHER SOURCE(S): MARPAT 134:320871
 AB Compds. which are antagonists of strong PPAR- γ agonists, such as rosiglitazone, and are also partial agonists of the PPAR- γ receptor, are active agents for correcting or reducing obesity. For example, 1-(p-chlorobenzyl)-5-chloro-3-thiophenylindole-2-carboxylic acid, is characterized as being a potent and selective ligand for PPAR- γ which has partial agonist (<30 maximal effects relative to rosiglitazone) and antagonist activity in cell-free and cell-based assays for the PPAR- γ receptor. The compd. is a potent agent for reducing obesity and insulin resistance in fat-fed C57BL/6J mice. This compd. and other PPAR- γ antagonists/partial agonists and pharmaceutically acceptable salts are effective in the treatment of obesity and related disorders, such as diabetes, insulin resistance, hyperlipidemia, atherosclerosis, inflammation and cancer.

IT 118414-59-8

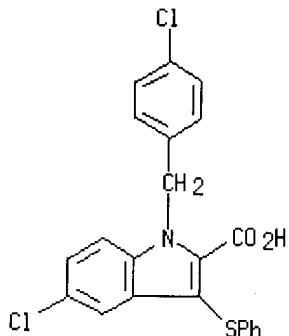
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(compns. contg. PPAR- γ receptor antagonists/partial agonists for treatment of obesity and related disorders)

RN 118414-59-8 HCPLUS

CN 1H-Indole-2-carboxylic acid, 5-chloro-1-[(4-chlorophenyl)methyl]-3-

(phenylthio)- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 2 OF 2 HCPLUS COPYRIGHT 2004 ACS on STN

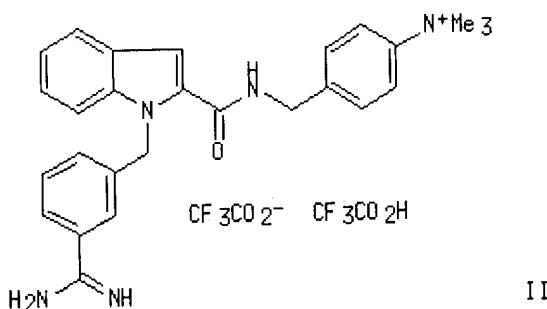
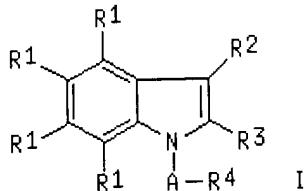
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| Full Text | Citing References |
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ACCESSION NUMBER: 1999:460399 HCPLUS
 DOCUMENT NUMBER: 131:87814
 TITLE: Indole derivatives as inhibitors of factor Xa, and their preparation and use as anticoagulants
 INVENTOR(S): Defossa, Elisabeth; Heinelt, Uwe; Klingler, Otmar; Zoller, Gerhard; Al-Obeidi, Fahad; Walser, Armin; Wildgoose, Peter; Matter, Hans
 PATENT ASSIGNEE(S): Hoechst Marion Roussel Deutschland GmbH, Germany
 SOURCE: PCT Int. Appl., 199 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|-------------------|----------|
| WO 9933800 | A1 | 19990708 | WO 1998-EP8030 | 19981210 |
| W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | | |
| CA 2316172 | AA | 19990708 | CA 1998-2316172 | 19981210 |
| AU 9920528 | A1 | 19990719 | AU 1999-20528 | 19981210 |
| AU 743881 | B2 | 20020207 | | |
| BR 9814340 | A | 20001003 | BR 1998-14340 | 19981210 |
| EP 1042287 | A1 | 20001011 | EP 1998-965244 | 19981210 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, SI, FI | | | | |
| TR 200001954 | T2 | 20001221 | TR 2000-200001954 | 19981210 |
| JP 2001527066 | T2 | 20011225 | JP 2000-526484 | 19981210 |
| NZ 505370 | A | 20020628 | NZ 1998-505370 | 19981210 |
| RU 2225397 | C2 | 20040310 | RU 2000-119774 | 19981210 |
| ZA 9811759 | A | 19990728 | ZA 1998-11759 | 19981222 |

| | | | |
|-----------------------------|---------------------------|--------------------------------|----------------------|
| NO 2000003057 US 6337344 | A 20000818 B1 20020108 | NO 2000-3057 US 2000-582344 | 20000614 20000814 |
| PRIORITY APPLN. INFO.: | | EP 1997-122901 | A 19971224 |
| | | WO 1998-EP8030 | W 19981210 |

OTHER SOURCE(S): MARPAT 131:87814
GI



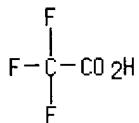
AB The invention relates to the inhibition of blood clotting proteins, and more particularly, to indole derivs. or their physiol. acceptable salts which effect this, having formula I [R1 groups = H, halo, alkyl, CF₃, (un)substituted Ph or phenylalkoxy, etc., with ≥2 of R1 being H; ≥1 of R2 and R3 = (CH₂)₀₋₂CO₂H or derivs., other = H, F, Cl, Br, or alkyl; or R₂R₃ = CH₂CH₂N(COPh)CH₂ or analogs; A = bond, alk(en/yn)ylene, CO, SO, SO₂, etc.; R₄ = (un)substituted Ph, pyridyl, or other heterocyclyl]. I are inhibitors of the blood clotting enzyme factor Xa. The invention also relates to processes for the prepn. of I, to methods of inhibiting factor Xa activity and blood clotting, to use of I in the treatment and prophylaxis of assocd. (e.g., thromboembolic) diseases, and to the use of I in the prepn. of related medicaments. The invention further relates to compns. contg. I, in particular pharmaceutical compns. contg. a compd. I and pharmaceutically acceptable carriers and/or auxiliary substances. Over 160 compds. I were prep'd. For instance, 1H-indole-2-carboxylic acid Et ester underwent a 5-step sequence to give title salt II. This prepn. involved (1) N-alkylation with 3-cyanobenzyl bromide, (2) alk. hydrolysis of the ester, (3) amidation with 4-(Me₂N)C₆H₄CH₂NH₂.2HCl, (4) conversion of the nitrile to a thioamide, and (5) quaternization at dimethylamino, and ammonolysis of the thioamide to an amidine. In an assay using human factor Xa in vitro, II had a Ki value of 0.090 μM.

IT 229950-28-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (target compd.; prepn. of indole derivs. as inhibitors of factor Xa)

RN 229950-28-1 HCPLUS
CN Pyridinium, 4-[[[[1-[[3-(aminoiminomethyl)phenyl]methyl]-3-(methoxycarbonyl)-1H-indol-2-yl]carbonyl]amino]methyl]-1-methyl-, salt with trifluoroacetic acid (1:1), mono(trifluoroacetate) (9CI) (CA INDEX

NAME)

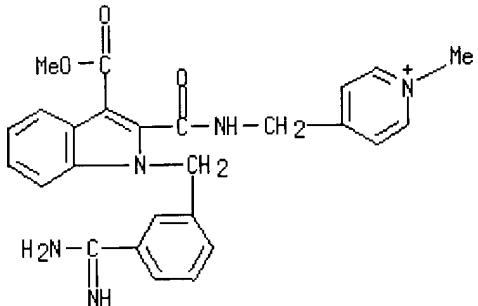
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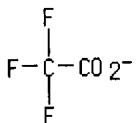
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CRN 229950-27-0
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CM 3

CRN 229950-26-9
CMF C26 H26 N5 O3

CM 4

CRN 14477-72-6
CMF C2 F3 O2

REFERENCE COUNT:

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THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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FILE 'REGISTRY' ENTERED AT 19:21:16 ON 22 JUN 2004

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| L3 | 579 S L1 FULL |

FILE 'HCAPLUS' ENTERED AT 19:22:04 ON 22 JUN 2004

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 L5 6 S L4 AND ARTHRITIS?
 L6 1 S L5 AND FAULL, A?/AU
 L7 5 S L5 NOT L6
 L8 33 S L4 NOT L5
 L9 0 S L8 AND GLOMERULAR?
 L10 0 S L8 AND LUNG () FIBROSIS?
 L11 2 S L8 AND RESTENOSIS?
 L12 0 S L11 AND FAULL, A?/AU
 L13 0 S L11 AND KETTLE, J?/AU

=> s 18 and alveolitis?
 677 ALVEOLITIS?
 L14 0 L8 AND ALVEOLITIS?

=> s 18 and asthma?
 25401 ASTHMA?
 L15 3 L8 AND ASTHMA?

=> s l15 and faull, a?/au
 34 FAULL, A?/AU
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=> s 11 and kettle, j?/au
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 Substance data SEARCH and crossover from CAS REGISTRY in progress...
 Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

SAMPLE SEARCH INITIATED 19:24:50 FILE 'REGISTRY'
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11.3% PROCESSED 1000 ITERATIONS
 INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
 SEARCH TIME: 00.00.01

4 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
 BATCH **COMPLETE**
 PROJECTED ITERATIONS: 171619 TO 182901
 PROJECTED ANSWERS: 352 TO 1066

L17 4 SEA SSS SAM L1

L18 4 L17

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 L19 1 L18 AND KETTLE, J?/AU

| | SINCE FILE ENTRY | TOTAL SESSION |
|----------------------|---------------------|------------------|
| => file hcaplus | | |
| COST IN U.S. DOLLARS | | |
| FULL ESTIMATED COST | 2.36 | 208.26 |

| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION |
|--|------------------|---------------|
| CA SUBSCRIBER PRICE | 0.00 | -5.54 |

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FILE COVERS 1907 - 22 Jun 2004 VOL 140 ISS 26
 FILE LAST UPDATED: 21 Jun 2004 (20040621/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

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(FILE 'HOME' ENTERED AT 19:21:10 ON 22 JUN 2004)

FILE 'REGISTRY' ENTERED AT 19:21:16 ON 22 JUN 2004

L1 STRUCTURE uploaded
 L2 4 S L1
 L3 579 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 19:22:04 ON 22 JUN 2004

L4 39 S L3/THU
 L5 6 S L4 AND ARTHRITIS?
 L6 1 S L5 AND FAULL, A?/AU
 L7 5 S L5 NOT L6
 L8 33 S L4 NOT L5
 L9 0 S L8 AND GLOMERULAR?
 L10 0 S L8 AND LUNG () FIBROSIS?
 L11 2 S L8 AND RESTENOSIS?
 L12 0 S L11 AND FAULL, A?/AU
 L13 0 S L11 AND KETTLE, J?/AU
 L14 0 S L8 AND ALVEOLITIS?
 L15 3 S L8 AND ASTHMA?
 L16 0 S L15 AND FAULL, A?/AU
 S L1 AND KETTLE, J?/AU

FILE 'REGISTRY' ENTERED AT 19:24:50 ON 22 JUN 2004

L17 4 S L1

FILE 'HCAPLUS' ENTERED AT 19:24:51 ON 22 JUN 2004

L18 4 S L17
 L19 1 S L18 AND KETTLE, J?/AU

FILE 'HCAPLUS' ENTERED AT 19:25:00 ON 22 JUN 2004

=> d 119, ibib abs fhitstr, 1

L19 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2004 ACS on STN

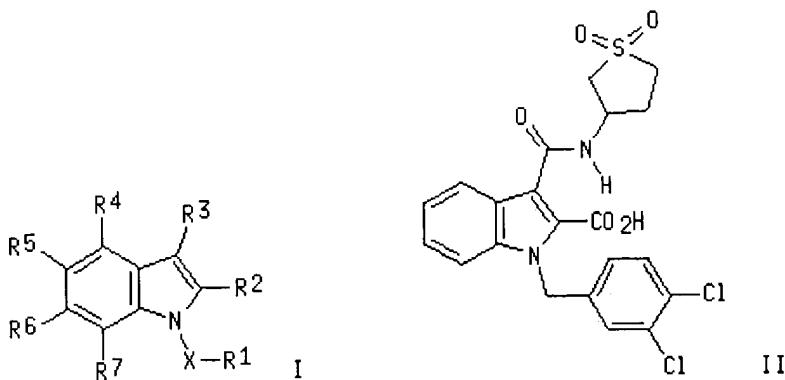
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| Full Text | Citing References |
|-----------|-------------------|

ACCESSION NUMBER: 2000:553556 HCAPLUS
 DOCUMENT NUMBER: 133:150463
 TITLE: Preparation of 3-substituted indole-2-carboxylic acids
 for the inhibition of monocyte chemoattractant
 protein-1 and/or RANTES induced chemotaxis
 INVENTOR(S): Faull, Alan Wellington; Kettle, Jason
 PATENT ASSIGNEE(S): AstraZeneca UK Limited, UK
 SOURCE: PCT Int. Appl., 72 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|--|------|----------|-----------------|------------|
| WO 2000046199 | A2 | 20000810 | WO 2000-GB284 | 20000131 |
| WO 2000046199 | A3 | 20001130 | | |
| W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | | |
| CA 2355734 | AA | 20000810 | CA 2000-2355734 | 20000131 |
| BR 2000008015 | A | 20011106 | BR 2000-8015 | 20000131 |
| EP 1173421 | A2 | 20020123 | EP 2000-901747 | 20000131 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO | | | | |
| JP 2002536362 | T2 | 20021029 | JP 2000-597270 | 20000131 |
| ZA 2001005017 | A | 20020919 | ZA 2001-5017 | 20010619 |
| NO 2001003768 | A | 20011001 | NO 2001-3768 | 20010801 |
| PRIORITY APPLN. INFO.: | | | GB 1999-2455 | A 19990205 |
| | | | WO 2000-GB284 | W 20000131 |

OTHER SOURCE(S) : MARPAT 133:150463

GI



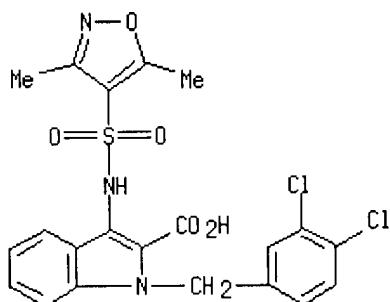
AB The title compds. [I; X = CH₂, SO₂; R₁ = (un)substituted aryl, heteroaryl; R₂ = CO₂H, CN, COCH₂OH, etc.; R₃ = OR₁₅ (wherein R₁₅ = substituted alkyl or cycloalkyl, (un)substituted heteroaryl), S(O)_qR₁₅ (q = 0-2), (CH₂)_sCO₂H (s = 0-4), etc.; R₄-R₇ = H, (un)substituted hydrocarbyl, heterocyclyl, etc.] and their pharmaceutically acceptable salts, amides or esters, useful in the prepn. of a medicament for the inhibition of monocyte chemoattractant protein-1 and/or RANTES induced chemotaxis, were prepd. and formulated. Thus, hydrolysis of the corresponding ester afforded 93% II which showed IC₅₀ of 6.86 μM against hMCP-1 receptor binding.

IT **287725-15-9P**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (prepn. of 3-substituted indole-2-carboxylic acids for the inhibition of monocyte chemoattractant protein-1 and/or RANTES induced chemotaxis)

RN 287725-15-9 HCAPLUS

CN 1H-Indole-2-carboxylic acid, 1-[(3,4-dichlorophenyl)methyl]-3-[(3,5-dimethyl-4-isoxazolyl)sulfonyl]amino]- (9CI) (CA INDEX NAME)



=> d his

(FILE 'HOME' ENTERED AT 19:21:10 ON 22 JUN 2004)

FILE 'REGISTRY' ENTERED AT 19:21:16 ON 22 JUN 2004

L1 STRUCTURE UPLOADED
 L2 4 S L1
 L3 579 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 19:22:04 ON 22 JUN 2004

L4 39 S L3/THU
 L5 6 S L4 AND ARTHRITIS?
 L6 1 S L5 AND FAULL, A?/AU

L7 5 S L5 NOT L6
 L8 33 S L4 NOT L5
 L9 0 S L8 AND GLOMERULAR?
 L10 0 S L8 AND LUNG () FIBROSIS?
 L11 2 S L8 AND RESTENOSIS?
 L12 0 S L11 AND FAULL, A?/AU
 L13 0 S L11 AND KETTLE, J?/AU
 L14 0 S L8 AND ALVEOLITIS?
 L15 3 S L8 AND ASTHMA?
 L16 0 S L15 AND FAULL, A?/AU
 S L1 AND KETTLE, J?/AU

FILE 'REGISTRY' ENTERED AT 19:24:50 ON 22 JUN 2004

L17 4 S L1

FILE 'HCAPLUS' ENTERED AT 19:24:51 ON 22 JUN 2004

L18 4 S L17
 L19 1 S L18 AND KETTLE, J?/AU

FILE 'HCAPLUS' ENTERED AT 19:25:00 ON 22 JUN 2004

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 L20 3 L15 NOT L19

=> d l20, ibib abs fhitstr, 1-3

L20 ANSWER 1 OF 3 HCAPLUS COPYRIGHT 2004 ACS on STN

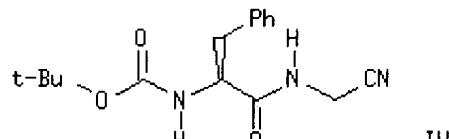
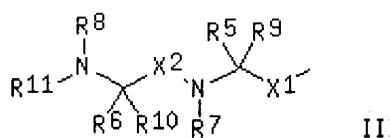
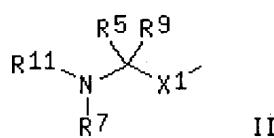
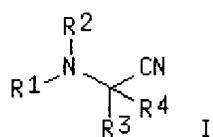
| | |
|--|--|
| <input type="checkbox"/> Full Text <input type="checkbox"/> Citing References | 2000:666700 HCAPLUS 133:252170 Preparation of novel N-cyanomethyl amides as protease inhibitors Bryant, Clifford M.; Bunin, Barry A.; Kraynack, Erica A.; Patterson, John W. Axys Pharmaceuticals, Inc., USA PCT Int. Appl., 137 pp. CODEN: PIXXD2 |
| DOCUMENT NUMBER: | 2000:666700 HCAPLUS |
| TITLE: | Preparation of novel N-cyanomethyl amides as protease inhibitors |
| INVENTOR(S): | Bryant, Clifford M.; Bunin, Barry A.; Kraynack, Erica A.; Patterson, John W. |
| PATENT ASSIGNEE(S): | Axys Pharmaceuticals, Inc., USA |
| SOURCE: | PCT Int. Appl., 137 pp. |
| DOCUMENT TYPE: | Patent |
| LANGUAGE: | English |
| FAMILY ACC. NUM. COUNT: | 2 |

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---------------|--|----------|-----------------|----------|
| WO 2000055125 | A2 | 20000921 | WO 2000-US6747 | 20000315 |
| WO 2000055125 | A3 | 20010426 | | |
| W: | AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | |
| RW: | GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | |
| BR 2000009042 | A | 20011226 | BR 2000-9042 | 20000315 |
| EP 1178958 | A2 | 20020213 | EP 2000-916343 | 20000315 |
| EP 1178958 | B1 | 20040218 | | |
| R: | AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, | | | |

| IE, SI, LT, LV, FI, RO | | | |
|-------------------------------|----|----------|---------------------------|
| TR 200103337 | T2 | 20020321 | TR 2001-20010333720000315 |
| TR 200103390 | T2 | 20020521 | TR 2001-20010339020000315 |
| US 6455502 | B1 | 20020924 | US 2000-526090 20000315 |
| TR 200201874 | T2 | 20021021 | TR 2002-20020187420000315 |
| US 6476026 - <i>nd</i> | B1 | 20021105 | US 2000-526485 20000315 |
| JP 2002539191 | T2 | 20021119 | JP 2000-605556 20000315 |
| EE 200100485 | A | 20030217 | EE 2001-485 20000315 |
| NZ 514234 | A | 20040227 | NZ 2000-514234 20000315 |
| AT 259782 | E | 20040315 | AT 2000-916343 20000315 |
| ZA 2001007494 | A | 20020911 | ZA 2001-7494 20010911 |
| ZA 2001007495 | A | 20020911 | ZA 2001-7495 20010911 |
| NO 2001004485 | A | 20011105 | NO 2001-4485 20010914 |
| BG 106003 | A | 20020628 | BG 2001-106003 20011010 |
| HR 2001000738 | A1 | 20021231 | HR 2001-738 20011012 |
| US 2002086996- <i>nd</i> | A1 | 20020704 | US 2001-17851 20011214 |
| US 6593327 - <i>nd</i> | B2 | 20030715 | |
| US 2003096796- <i>nd</i> | A1 | 20030522 | US 2002-205600 20020724 |
| US 2003119788 <i>nd</i> | A1 | 20030626 | US 2002-241001 20020909 |
| <u>PRIORITY APPLN. INFO.:</u> | | | |
| US 1999-124420P P 19990315 | | | |
| US 2000-526090 A1 20000315 | | | |
| US 2000-526485 A3 20000315 | | | |
| WO 2000-US6747 W 20000315 | | | |

OTHER SOURCE(S) : MARPAT 133:252170
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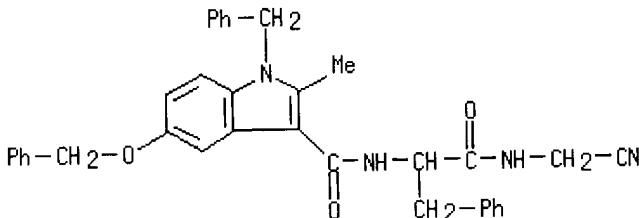
AB The title compds. [I; R1 = II, III (wherein X1, X2 = CO, CH₂SO₂; R5, R6 = H, alkyl; R7, R8 = H, alkyl, etc.; R9, R10 = alkyl optionally substituted with CN, halo, NO₂, etc.; R11 = X₅X₆R18; X₅ = CO, COCO, SO₂; X₆ = a bond, O, NH, N(alkyl); R18 = alkyl optionally substituted with CN, halo, NO₂, etc.); R2 = H, alkyl, etc.; R3 = H, alkyl, etc.; R4 = H, alkyl optionally substituted with CN, halo, NO₂, etc.; R4 and R2 taken together form trimethylene, tetramethylene, phenylene-1,2-dimethylene, optionally substituted with hydroxy, oxo or methylene; R4 and R3 together with the carbon atom to which both are attached form cycloalkylene, heterocycloalkylene], useful for treating diseases assocd. with cysteine protease activity, particularly diseases assocd. with activity of cathepsins B, K, L or S such as inflammation and **asthma**, were prepd. and formulated. Thus, reacting (2S)-tert-butoxycarbonylamino-3-phenylpropionic acid with aminoacetonitrile.HCl in the presence of Et₃N DMF and MeCN afforded the amide (1S)-IV. Biol. data for compds. I were given.

IT 294640-68-9P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (prep. of novel N-cyanomethyl amides as protease inhibitors)

RN 294640-68-9 HCAPLUS

CN 1H-Indole-3-carboxamide, N-[2-[(cyanomethyl)amino]-2-oxo-1-(phenylmethyl)ethyl]-2-methyl-5-(phenylmethoxy)-1-(phenylmethyl)- (9CI)
(CA INDEX NAME)



L20 ANSWER 2 OF 3 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text Citing References

ACCESSION NUMBER:

1996:746234 HCAPLUS

DOCUMENT NUMBER:

126:18786

TITLE:

Indole derivatives as cGMP-PDE inhibitors

INVENTOR(S):

Oku, Teruo; Sawada, Kozo; Kuroda, Akio; Ohne, Kazuhiko; Nomoto, Atsushi; Hosogai, Naomi; Nakajima, Yoshimitsu; Nagashima, Akira; Sogabe, Keizo; Amura, Kouichi

PATENT ASSIGNEE(S):

Fujisawa Pharmaceutical Co, Ltd., Japan

SOURCE:

PCT Int. Appl., 211 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

1

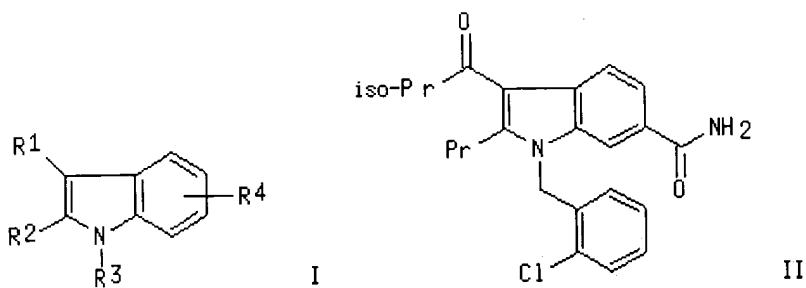
PATENT INFORMATION:

None of the Examples

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|------------------|------------|
| WO 9632379 | A1 | 19961017 | WO 1996-JP892 | 19960402 |
| CA 2217707 | AA | 19961017 | CA 1996-2217707 | 19960402 |
| AU 9651234 | A1 | 19961030 | AU 1996-51234 | 19960402 |
| AU 713460 | B2 | 19991202 | | |
| EP 820441 | A1 | 19980128 | EP 1996-907750 | 19960402 |
| EP 820441 | B1 | 20020626 | | |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI | | | | |
| CN 1187812 | A | 19980715 | CN 1996-194691 | 19960402 |
| JP 11503445 | T2 | 19990326 | JP 1996-530864 | 19960402 |
| AT 219765 | E | 20020715 | AT 1996-907750 | 19960402 |
| ES 2175079 | T3 | 20021116 | ES 1996-907750 | 19960402 |
| ZA 9602859 | A | 19961011 | ZA 1996-2859 | 19960410 |
| TW 420663 | B | 20010201 | TW 1996-85104519 | 19960416 |
| US 6069156 | A | 20000530 | US 1997-930597 | 19971210 |
| PRIORITY APPLN. INFO.: | | | | |
| <i>Take off</i> | | | | |
| | | | GB 1995-7432 | A 19950410 |
| | | | GB 1995-12560 | A 19950621 |
| | | | GB 1995-16136 | A 19950807 |
| | | | AU 1996-8294 | A 19960227 |
| | | | WO 1996-JP892 | W 19960402 |

OTHER SOURCE(S): MARPAT 126:18786

GI



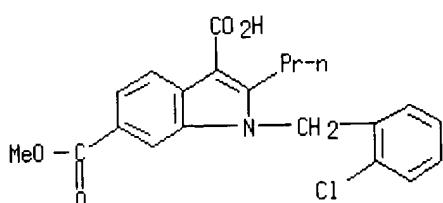
AB The invention relates to new indole derivs. I and their pharmaceutically acceptable salts [wherein R1 = H, halo, NO₂, CO₂H, protected CO₂H, acyl, (un)substituted alk(en)yl, etc.; R2 = H, halo, alkenyl, acyl, (un)substituted alkyl, etc.; R3 = (un)substituted alk(en)yl where the substituent is oxo, (un)substituted aryl, or heterocyclyl; R4 = CO₂H, protected CO₂H, acyl, cyano, amino, halo, etc.; R1 and R2 may form 4- to 7-membered carboxylic ring (un)substituted with oxo]. I are cyclic nucleotide-PDE inhibitors (specifically cGMP-PDE), and are useful for treating and preventing a variety of conditions, including angina, hypertension, renal failure, atherosclerosis, stroke, **asthma**, impotence, diabetic complications, and glaucoma. Almost 300 compds. I and numerous intermediates were prep'd. For example, Me 3-isobutyryl-2-propylindole-6-carboxylate (prepn. given) was N-benzylated by 2-chlorobenzyl bromide using NaH in DMF. The product underwent sapon. with NaOH in aq. EtOH, followed by amidation of the resultant acid using EDC, HOBT, and aq. NH₃ to give title amide II. II inhibited human platelet cGMP-PDE in vitro with IC₅₀ <100 nM. I were also active in a variety of other bioassays, including relaxation of isolated rat aorta, inhibition of vascular smooth muscle cell proliferation, inhibition of vasopressin-induced vasospasm, the cyclosporin and FK506 nephritis models, the diabetic glomerulosclerosis model, and several animal impotence models.

IT 184149-02-8P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); **THU (Therapeutic use)**; **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses) (prepn. of indole derivs. as cGMP-PDE inhibitors)

RN 184149-02-8 HCAPLUS

CN 1H-Indole-3,6-dicarboxylic acid, 1-[(2-chlorophenyl)methyl]-2-propyl-6-methyl ester (9CI) (CA INDEX NAME)



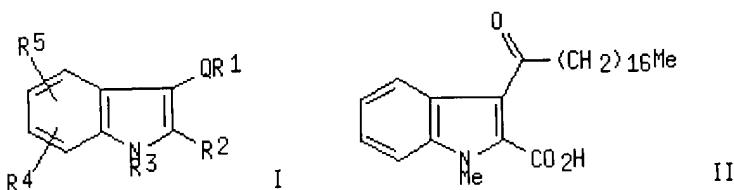
L20 ANSWER 3 OF 3 HCAPLUS COPYRIGHT 2004 ACS on STN

| | |
|-----------|-------------------|
| Full Text | Citing References |
|-----------|-------------------|

ACCESSION NUMBER: 1995:638471 HCAPLUS
DOCUMENT NUMBER: 123:32958

TITLE: Indole-2-alkanoic acids and their derivatives as
inhibitors of phospholipase A2.
INVENTOR(S): Lehr, Matthias
PATENT ASSIGNEE(S): Germany
SOURCE: Ger. Offen., 30 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

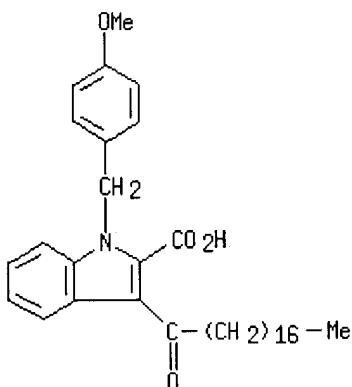
| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|------------------|-----------------|----------|
| DE 4338770 | A1 | 19950518 | DE 1993-4338770 | 19931112 |
| WO 9513266 | A1 | 19950518 | WO 1994-DE1121 | 19940920 |
| W: AM, AU, BB, BG, BR, BY, CA, CN, CZ, EE, FI, GE, HU, JP, KG, KP, KR, KZ, LK, LR, LT, LV, MD, MG, MN, NO, NZ, PL, RO, RU, SI, SK, TJ, TT, UA, US, UZ, VN | | | | |
| RW: KE, MW, SD, SZ, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG | | | | |
| AU 9476907 | A1 | 19950529 | AU 1994-76907 | 19940920 |
| PRIORITY APPLN. INFO.: | | | DE 1993-4338770 | 19931112 |
| | | | WO 1994-DE1121 | 19940920 |
| OTHER SOURCE(S) : | | MARPAT 123:32958 | | |
| C1 | | | | |



AB Title compds. I [R1 = X, (un)substituted aryl, -X-aryl; X = C1-19 alk(en/yn)yl optionally interrupted by O; R2 = CO2H, -Y-CO2H, Tz, -Y-Tz; Y = C1-8 alk(en)yl optionally interrupted by O; Tz = 1H- or 2H-tetrazol-5-yl; R3 = H, Z (Z = C1-20 alk(en/yn)yl optionally interrupted by O), (un)substituted aryl or -Z-aryl, or Z (un)substituted by OH, acyloxy, SH, acylthio, NH2, or acylamino; Q = CO, CH2, (acylamino)methylene; R4, R5 = H, as given for Z, halo, CF3, OH, cyano, many others] and their pharmaceutical salts and esters are claimed. The compds. are inhibitors of phospholipase A2 (PLA2), and are claimed useful for treatment or prevention of inflammation, allergy, **asthma**, psoriasis, and endotoxin shock. For example, acylation of indole-2-carboxylic acid Et ester with octadecanoic acid in CH2C12 in the presence of polyphosphoric acid and (CF3CO)2O gave 42% 3-octadecanoyl deriv., which was N-alkylated by p-MeC6H4SO3Me under phase-transfer conditions (75%) and hydrolyzed by aq. KOH in refluxing EtOH (80%) to give title compd. II. In a test for inhibition of PLA2 using bovine platelets in vitro, II at 10 μ M gave 61% inhibition, vs. only 42% for the known inhibitor (S)-N-hexadecyl-2-pyrrolidinecarboxamide.

IT **164160-85-4P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); **THU (Therapeutic use); THU (Therapeutic use);** BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses) (prep. of indolealkanoic acids as phospholipase A2 inhibitors)

RN 164160-85-4 HCAPLUS
CN 1H-Indole-2-carboxylic acid, 1-[(4-methoxyphenyl)methyl]-3-(1-oxooctadecyl)- (9CI) (CA INDEX NAME)



=> d his

(FILE 'HOME' ENTERED AT 19:21:10 ON 22 JUN 2004)

FILE 'REGISTRY' ENTERED AT 19:21:16 ON 22 JUN 2004

L1 STRUCTURE UPLOADED
L2 4 S L1
L3 579 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 19:22:04 ON 22 JUN 2004

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| L4 | 39 S L3/THU |
| L5 | 6 S L4 AND ARTHRITIS? |
| L6 | 1 S L5 AND FAULL, A?/AU |
| L7 | 5 S L5 NOT L6 |
| L8 | 33 S L4 NOT L5 |
| L9 | 0 S L8 AND GLOMERULAR? |
| L10 | 0 S L8 AND LUNG () FIBROSIS? |
| L11 | 2 S L8 AND RESTENOSIS? |
| L12 | 0 S L11 AND FAULL, A?/AU |
| L13 | 0 S L11 AND KETTLE, J?/AU |
| L14 | 0 S L8 AND ALVEOLITIS? |
| L15 | 3 S L8 AND ASTHMA? |
| L16 | 0 S L15 AND FAULL, A?/AU |
| | S L1 AND KETTLE, J?/AU |

L17 4 S L1 FILE 'REGISTRY' ENTERED AT 19:24:50 ON 22 JUN 2004

FILE 'HCAPLUS' ENTERED AT 19:24:51 ON 22 JUN 2004
L18 4 S L17
L19 1 S L18 AND KETTLE, J?/AU

FILE 'HCAPLUS' ENTERED AT 19:25:00 ON 22 JUN 2004
L20 3 S L15 NOT L19

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39766 ATHEROSCLEROSIS?

L22 1 L21 AND ATHEROSCLEROSIS?

=> s 122 and faull, a?/au

34 FAULL, A?/AU

L23 0 L22 AND FAULL, A?/AU

=> s 122 and kettle, j?/au

39 KETTLE, J?/AU

L24 0 L22 AND KETTLE, J?/AU

=> d 122, ibib abs fhitstr, 1

L22 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Citing
 Text References

ACCESSION NUMBER: 2001:319722 HCAPLUS
 DOCUMENT NUMBER: 134:320871
 TITLE: Pharmaceuticals for treating obesity containing
 antagonists and partial agonists of PPAR- γ
 INVENTOR(S): Berger, Joel P.; Doepper, Thomas W.; Leibowitz, Mark;
 Moller, David E.; Mosley, Ralph T.; Tolman, Richard
 L.; Ventre, John; Zhang, Bei B.; Zhou, Gaochao
 PATENT ASSIGNEE(S): Merck & Co., Inc., USA
 SOURCE: PCT Int. Appl., 49 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|--|------|----------|-----------------|----------|
| WO 2001030343 | A1 | 20010503 | WO 2000-US28924 | 20001019 |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | | |
| EP 1284728 | A1 | 20030226 | EP 2000-973670 | 20001019 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL | | | | |
| JP 2003525217 | T2 | 20030826 | JP 2001-532763 | 20001019 |
| US 2003032581 | A1 | 20030213 | US 2002-241106 | 20020911 |
| <u>PRIORITY APPLN. INFO.:</u> | | | | |
| US 1999-161225P | | | | |
| P 19991022 | | | | |
| US 2000-691955 | | | | |
| A3 20001019 | | | | |
| WO 2000-US28924 | | | | |
| W 20001019 | | | | |

OTHER SOURCE(S): MARPAT 134:320871

AB Compds. which are antagonists of strong PPAR- γ agonists, such as rosiglitazone, and are also partial agonists of the PPAR- γ receptor, are active agents for correcting or reducing obesity. For example, 1-(p-chlorobenzyl)-5-chloro-3-thiophenylindole-2-carboxylic acid, is characterized as being a potent and selective ligand for PPAR- γ which has partial agonist (<30 maximal effects relative to rosiglitazone) and antagonist activity in cell-free and cell-based assays for the PPAR- γ receptor. The compd. is a potent agent for reducing obesity

and insulin resistance in fat-fed C57BL/6J mice. This compd. and other PPAR- γ antagonists/partial agonists and pharmaceutically acceptable salts are effective in the treatment of obesity and related disorders, such as diabetes, insulin resistance, hyperlipidemia, **atherosclerosis**, inflammation and cancer.

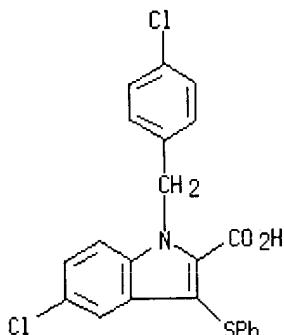
IT 118414-59-8

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(compns. contg. PPAR- γ receptor antagonists/partial agonists for treatment of obesity and related disorders)

RN 118414-59-8 HCAPLUS

CN 1H-Indole-2-carboxylic acid, 5-chloro-1-[(4-chlorophenyl)methyl]-3-(phenylthio)- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

5

THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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(FILE 'HOME' ENTERED AT 19:21:10 ON 22 JUN 2004)

FILE 'REGISTRY' ENTERED AT 19:21:16 ON 22 JUN 2004

L1 STRUCTURE uploaded
 L2 4 S L1
 L3 579 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 19:22:04 ON 22 JUN 2004

L4 39 S L3/THU
 L5 6 S L4 AND ARTHRITIS?
 L6 1 S L5 AND FAULL, A?/AU
 L7 5 S L5 NOT L6
 L8 33 S L4 NOT L5
 L9 0 S L8 AND GLOMERULAR?
 L10 0 S L8 AND LUNG () FIBROSIS?
 L11 2 S L8 AND RESTENOSIS?
 L12 0 S L11 AND FAULL, A?/AU
 L13 0 S L11 AND KETTLE, J?/AU
 L14 0 S L8 AND ALVEOLITIS?
 L15 3 S L8 AND ASTHMA?
 L16 0 S L15 AND FAULL, A?/AU
 S L1 AND KETTLE, J?/AU

FILE 'REGISTRY' ENTERED AT 19:24:50 ON 22 JUN 2004

L17 4 S L1

FILE 'HCAPLUS' ENTERED AT 19:24:51 ON 22 JUN 2004
 L18 4 S L17
 L19 1 S L18 AND KETTLE, J?/AU

FILE 'HCAPLUS' ENTERED AT 19:25:00 ON 22 JUN 2004
 L20 3 S L15 NOT L19
 L21 30 S L8 NOT L20
 L22 1 S L21 AND ATHEROSCLEROSIS?
 L23 0 S L22 AND FAULL, A?/AU
 L24 0 S L22 AND KETTLE, J?/AU

=> s 121 not 122
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=> s 125 and skin?
 213767 SKIN?
 L26 2 L25 AND SKIN?

=> s 126 and faull, a?/au
 34 FAULL, A?/AU
 L27 0 L26 AND FAULL, A?/AU

=> s 125 and kettle, j?/au
 39 KETTLE, J?/AU
 L28 3 L25 AND KETTLE, J?/AU

=> s 126 and kettle, j?/au
 39 KETTLE, J?/AU
 L29 0 L26 AND KETTLE, J?/AU

=> d 126, ibib abs fhitstr, 1-2

L26 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2004 ACS on STN

| | |
|-----------|-------------------|
| Full Text | Citing References |
|-----------|-------------------|

ACCESSION NUMBER: 2003:551494 HCAPLUS
 DOCUMENT NUMBER: 139:101027
 TITLE: Preparation of mercaptoethyl indolecarboxylic acids as NAALAdase inhibitors for treating and diagnosing glutamate abnormalities, neurological and other disorders
 INVENTOR(S): Tsukamoto, Takashi; Grella, Brian; Majer, Pavel
 PATENT ASSIGNEE(S): Guilford Pharmaceuticals Inc., USA
 SOURCE: PCT Int. Appl., 173 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|-----------------|----------|
| WO 2003057670 | A2 | 20030717 | WO 2002-US37617 | 20021219 |
| WO 2003057670 | A3 | 20031106 | | |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, | | | | |

RU, TJ, TM

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

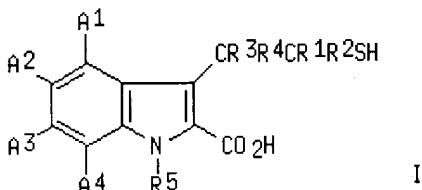
PRIORITY APPLN. INFO.:

US 2001-342764P P 20011228

OTHER SOURCE(S):

MARPAT 139:101027

GI



AB This invention relates to new indoles (shown as I; variables defined below; e.g. 3-(2-mercaptopethyl)-1H-indole-2-carboxylic acid), pharmaceutical compns. and diagnostic kits comprising such compds., and methods of using such compds. for inhibiting NAALAdase enzyme activity, detecting diseases where NAALAdase levels are altered, affecting neuronal activity, effecting TGF- β activity, inhibiting angiogenesis, and treating glutamate abnormalities, neuropathy, pain, compulsive disorders, prostate diseases, cancers and glaucoma. IC₅₀ values are tabulated for inhibition of NAALAdase by 12 examples of I. Many pharmacol. and therapeutic test results are reported for the following 6 compds. that are not covered by I: 2-[(2,3,4,5,6-pentafluorobenzyl)hydroxyphosphinyl]methylpentanedioic acid, 2-(3-sulfanylpropyl)pentanedioic acid, 2-(phosphonomethyl)pentanedioic acid, 2-(2-sulfanylethyl)pentanedioic acid, 3-carboxy- α -(3-mercaptopropyl)benzenepropanoic acid and 3-carboxy-5-(1,1-dimethylethyl)- α -(3-mercaptopropyl)benzenepropanoic acid. For I: A1, A2, A3 and A4 = H, C1-C9 alkyl, C2-C9 alkenyl, C2-C9 alkynyl, aryl, heteroaryl, carbocycle, heterocycle, C1-C9 alkoxy, C2-C9 alkenyloxy, phenoxy, benzyloxy, hydroxy, halo, nitro, cyano, isocyano, -COOR₆, -COR₆, -NR₆R₇, -SR₆, -SOR₆, -SO₂R₆, -SO₂(OR₆), -C(O)NR₆R₇, -C(O)NR₆(CH₂)_nCOOH, -NR₆C(O)R₇ or -(CH₂)_nCOOH, or any adjacent two of A1, A2, A3 and A4 form with the benzene ring a fused ring that is (un)satd., arom. or nonarom., and carbocyclic or heterocyclic, said heterocyclic ring contg. 1 or 2 O, N and/or S heteroatom(s); n is 1-3; R, R₁, R₂, R₃, R₄, R₅, R₆, R₇ = H, carboxy, C1-C9 alkyl, C2-C9 alkenyl, C2-C9 alkynyl, aryl, heteroaryl, carbocycle or heterocycle; and said alkyl, alkenyl, alkynyl, aryl, heteroaryl, carbocycle, heterocycle, alkoxy, alkenyloxy, phenoxy, benzyloxy and fused ring (un)substituted with \geq 1 substituent(s). Although the methods of prepn. are not claimed, 13 example prepn.s. are included.

IT **560131-44-4P**, 1-[(3-Carboxyphenyl)methyl]-3-(2-mercaptopethyl)-1H-indole-2-carboxylic acid

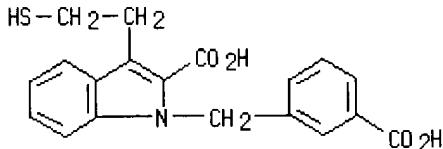
RL: DGN (Diagnostic use); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate and diagnosis agent; prepn. of mercaptoethyl indolecarboxylic acids as NAALAdase inhibitors for treating and diagnosing glutamate abnormalities and neurol. and other disorders)

RN **560131-44-4** HCAPLUS

CN 1H-Indole-2-carboxylic acid, 1-[(3-carboxyphenyl)methyl]-3-(2-

mercaptoethyl) - (9CI) (CA INDEX NAME)



L26 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2004 ACS on STN

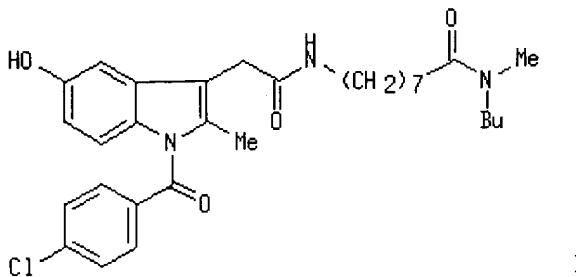
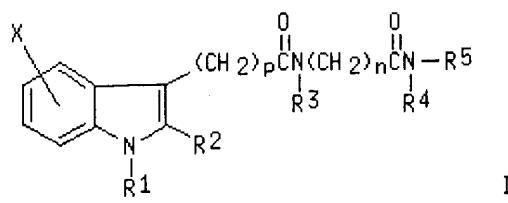
Full Text Citing References

ACCESSION NUMBER: 1995:994335 HCAPLUS
 DOCUMENT NUMBER: 124:86811
 TITLE: Novel indole derivatives useful to treat estrogen-related neoplasms and disorders
 INVENTOR(S): Bitonti, Alan J.; McDonald, Ian A.; Salituro, Francesco G.; Whitten, Jeffrey P.; Jarvi, Esa T.; Wright, Paul S.
 PATENT ASSIGNEE(S): Merrell Dow Pharmaceuticals Inc., USA
 SOURCE: PCT Int. Appl., 173 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|-----------------|-------------|
| WO 9522524 | A1 | 19950824 | WO 1995-US1372 | 19950131 |
| W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, ES, FI, GB, GE, HU, JP, KE, KG, KP, KR, KZ, LK, LT, LU, LV, MD, MG, MN, MW, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SI, SK, TJ, TT, UA, US, US, UZ, VN | | | | |
| RW: KE, MW, SD, SZ, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG | | | | |
| CA 2183731 | AA | 19950824 | CA 1995-2183731 | 19950131 |
| AU 9518373 | A1 | 19950904 | AU 1995-18373 | 19950131 |
| AU 680740 | B2 | 19970807 | | |
| EP 746544 | A1 | 19961211 | EP 1995-910164 | 19950131 |
| EP 746544 | B1 | 19980909 | | |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE | | | | |
| CN 1141627 | A | 19970129 | CN 1995-191750 | 19950131 |
| HU 76133 | A2 | 19970630 | HU 1996-2299 | 19950131 |
| JP 09509169 | T2 | 19970916 | JP 1995-521822 | 19950131 |
| JP 3536258 | B2 | 20040607 | | |
| AT 170839 | E | 19980915 | AT 1995-910164 | 19950131 |
| ES 2122555 | T3 | 19981216 | ES 1995-910164 | 19950131 |
| ZA 9501297 | A | 19951024 | ZA 1995-1297 | 19950216 |
| US 5877202 | A | 19990302 | US 1996-594505 | 19960131 |
| FI 9603272 | A | 19960821 | FI 1996-3272 | 19960821 |
| NO 9603483 | A | 19961022 | NO 1996-3483 | 19960821 |
| PRIORITY APPLN. INFO.: | | | US 1994-200057 | A2 19940222 |
| | | | US 1994-362046 | A2 19941222 |
| | | | WO 1995-US1372 | W 19950131 |

OTHER SOURCE(S): MARPAT 124:86811

GI



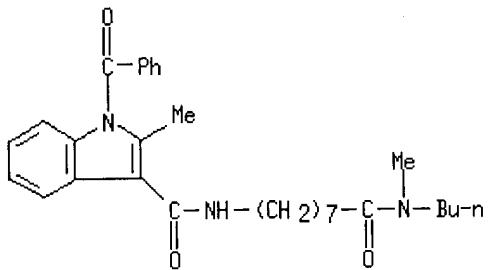
AB The invention relates to indole derivs. I [n = 1-12; p = 0, 1; X = 1-3 of H, halo, OH, alkyl, alkoxy, R₆CO₂; R₁ = H, alkyl, (un)substituted phenylalkyl, benzoyl, carbamoyl, etc.; R₂ = H, alkyl, (un)substituted Ph; R₃, R₄ = H, alkyl; R₅ = H, alkyl, Ph; or R₄R₅ = CH₂CH₂GCH₂CH₂; G = bond, NMe, CH₂, O; R₆ = alkyl, (un)substituted Ph; one of R₁-R₅ ≠ H when n = 1] and their pharmaceutically acceptable salts. I and salts are useful in down-regulating estrogen receptor expression. Also included are methods for the treatment or prophylaxis of neoplasms or of controlling neoplasm growth, esp. estrogen-dependent neoplasms such as those assocd. with breast, ovarian, and cervical tissue. Also provided is a method for treating autoimmune diseases. For example, reaction of 1-[5-methoxy-1-(4-chlorobenzoyl)-2-methyl-1H-indol-3-yl]acetic acid chloride with 8-aminoctanoic acid methylbutylamide [preps. given] in PhMe in the presence of (iso-Pr)₂NET, and demethylation of the phenolic Me ether with BBr₃ in CH₂Cl₂, gave the preferred compd. II [also named MDL 101,906]. The latter inhibited estradiol-dependent transcription of an estradiol-dependent luciferase reporter plasmid in MCF-7 human breast tumor cells with an IC₅₀ of 5.2 μM. Over 180 synthetic examples cover prepn. of I and intermediates, and 9 biol. examples cover a variety of tests of selected I, including relative binding affinities to estrogen receptor, depletion of receptor from tumor cells, and inhibition of cells including tamoxifen-resistant LY-2 cells (IC₅₀ of II = 4.7 μM).

IT **172595-48-1P**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses) (prepn. of indoles as estrogen-dependent antineoplastics)

RN **172595-48-1 HCPLUS**

CN 1H-Indole-3-carboxamide, 1-benzoyl-N-[8-(butylmethylamino)-8-oxooctyl]-2-methyl- (9CI) (CA INDEX NAME)



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(FILE 'HOME' ENTERED AT 19:21:10 ON 22 JUN 2004)

FILE 'REGISTRY' ENTERED AT 19:21:16 ON 22 JUN 2004

L1 STRUCTURE UPLOADED
 L2 4 S L1
 L3 579 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 19:22:04 ON 22 JUN 2004

L4 39 S L3/THU
 L5 6 S L4 AND ARTHRITIS?
 L6 1 S L5 AND FAULL, A?/AU
 L7 5 S L5 NOT L6
 L8 33 S L4 NOT L5
 L9 0 S L8 AND GLOMERULAR?
 L10 0 S L8 AND LUNG () FIBROSIS?
 L11 2 S L8 AND RESTENOSIS?
 L12 0 S L11 AND FAULL, A?/AU
 L13 0 S L11 AND KETTLE, J?/AU
 L14 0 S L8 AND ALVEOLITIS?
 L15 3 S L8 AND ASTHMA?
 L16 0 S L15 AND FAULL, A?/AU
 S L1 AND KETTLE, J?/AU

FILE 'REGISTRY' ENTERED AT 19:24:50 ON 22 JUN 2004

L17 4 S L1

FILE 'HCAPLUS' ENTERED AT 19:24:51 ON 22 JUN 2004

L18 4 S L17
 L19 1 S L18 AND KETTLE, J?/AU

FILE 'HCAPLUS' ENTERED AT 19:25:00 ON 22 JUN 2004

L20 3 S L15 NOT L19
 L21 30 S L8 NOT L20
 L22 1 S L21 AND ATHEROSCLEROSIS?
 L23 0 S L22 AND FAULL, A?/AU
 L24 0 S L22 AND KETTLE, J?/AU
 L25 29 S L21 NOT L22
 L26 2 S L25 AND SKIN?
 L27 0 S L26 AND FAULL, A?/AU
 L28 3 S L25 AND KETTLE, J?/AU
 L29 0 S L26 AND KETTLE, J?/AU

=> s 125 not 126

L30 27 L25 NOT L26

=> s 130 and multiple () sclerosis?

325687 MULTIPLE
 3005 MULTIPLES
 328373 MULTIPLE
 (MULTIPLE OR MULTIPLES)
 18498 SCLEOROSIS?
 10942 MULTIPLE (W) SCLEOROSIS?
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=> s 130 and inflamm? () bowel?
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=> s 130 and brain () trauma?
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 21566 BRAINS
 465094 BRAIN
 (BRAIN OR BRAINS)
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 826 BRAIN (W) TRAUMA?
 L33 1 L30 AND BRAIN (W) TRAUMA?

=> d 133, ibib abs fhitstr, 1

L33 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2004 ACS on STN

| | |
|----------------------------|---|
| Full Text | Citing References |
| ACCESSION NUMBER: | 1998:635621 HCAPLUS |
| DOCUMENT NUMBER: | 129:265475 |
| TITLE: | Indolecarboxamides, preparation thereof, pharmaceutical compositions, and methods of inhibiting calpain |
| INVENTOR(S): | Daines, Robert A.; Sham, Kelvin Kin-Cheong |
| PATENT ASSIGNEE(S): | Smithkline Beecham Corp., USA |
| SOURCE: | PCT Int. Appl., 17 pp. |
| DOCUMENT TYPE: | Patent |
| LANGUAGE: | English |
| FAMILY ACC. NUM. COUNT: | 1 |
| <u>PATENT INFORMATION:</u> | |

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|--|------|----------|-----------------|------------|
| WO 9841092 | A1 | 19980924 | WO 1998-US4873 | 19980313 |
| W: CA, JP, US | | | | |
| RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE | | | | |
| EP 1018878 | A1 | 20000719 | EP 1998-909146 | 19980313 |
| R: BE, CH, DE, ES, FR, GB, IT, LI, NL | | | | |
| JP 2001515508 | T2 | 20010918 | JP 1998-540629 | 19980313 |
| US 6214856 | B1 | 20010410 | US 1999-380317 | 19990830 |
| PRIORITY APPLN. INFO.: | | | US 1997-40589P | P 19970314 |
| | | | WO 1998-US4873 | W 19980313 |

OTHER SOURCE(S): MARPAT 129:265475
 AB Pharmaceutical compns. and methods of inhibiting calpain using indolecarboxamides are disclosed. The compns. and methods of the invention are useful in the treatment of e.g. neurodegenerative disorders, strokes, and traumatic brain injury. Prepn. of e.g. (S)-N-(1-formyl-2-phenylethyl)-1-methyl-2-indolecarboxamide is described, as are capsule and other formulations.

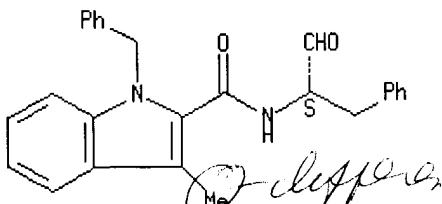
IT 213599-01-0P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (indolecarboxamides, prep., pharmaceutical compns., and methods of inhibiting calpain)

RN 213599-01-0 HCAPLUS

CN 1H-Indole-2-carboxamide, N-[(1S)-1-formyl-2-phenylethyl]-3-methyl-1-(phenylmethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT:

2

THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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(FILE 'HOME' ENTERED AT 19:21:10 ON 22 JUN 2004)

FILE 'REGISTRY' ENTERED AT 19:21:16 ON 22 JUN 2004

L1 STRUCTURE uploaded
 L2 4 S L1
 L3 579 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 19:22:04 ON 22 JUN 2004

L4 39 S L3/THU
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 L10 0 S L8 AND LUNG () FIBROSIS?
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 L13 0 S L11 AND KETTLE, J?/AU
 L14 0 S L8 AND ALVEOLITIS?
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 L16 0 S L15 AND FAULL, A?/AU
 S L1 AND KETTLE, J?/AU

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L17 4 S L1

FILE 'HCAPLUS' ENTERED AT 19:24:51 ON 22 JUN 2004

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 L19 1 S L18 AND KETTLE, J?/AU

FILE 'HCAPLUS' ENTERED AT 19:25:00 ON 22 JUN 2004

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 L21 30 S L8 NOT L20
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 L23 0 S L22 AND FAULL, A?/AU

L24 0 S L22 AND KETTLE, J?/AU
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 L27 0 S L26 AND FAULL, A?/AU
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 57074 ISCHEMIA?
 L35 1 L34 AND ISCHEMIA?

=> d l35, ibib abs fhitstr, 1

L35 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2004 ACS on STN

| | |
|-----------|-------------------|
| Full Text | Citing References |
|-----------|-------------------|

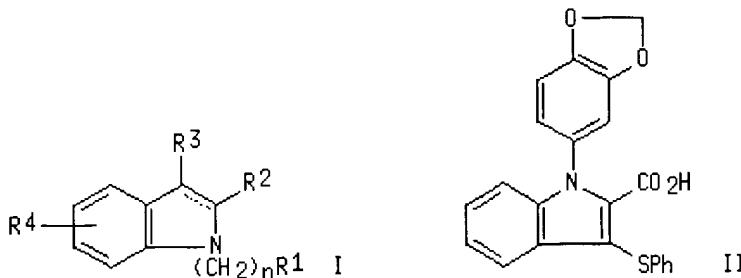
ACCESSION NUMBER: 1996:87548 HCAPLUS
 DOCUMENT NUMBER: 124:260835
 TITLE: Indole-2-carboxylic acids as nonpeptide endothelin antagonists
 INVENTOR(S): Berryman, Kent A.; Bunker, Amy M.; Doherty, Annette M.; Edmunds, Jeremy J.
 PATENT ASSIGNEE(S): Warner-Lambert Co., USA
 SOURCE: U.S., 12 pp.
 CODEN: USXXAM

Wolfe

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|-----------------|----------|
| US 5482960 | A | 19960109 | US 1994-339381 | 19941114 |
| WO 9615125 | A1 | 19960523 | WO 1995-US12672 | 19951002 |
| W: CA, EE, JP, LT, LV, MX, SI RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE | | | | |
| CA 2202051 | AA | 19960523 | CA 1995-2202051 | 19951002 |
| EP 790993 | A1 | 19970827 | EP 1995-937320 | 19951002 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE | | | | |
| JP 10508843 | T2 | 19980902 | JP 1995-516037 | 19951002 |
| <u>PRIORITY APPLN. INFO.:</u> | | | | |
| US 1994-339381 19941114 | | | | |
| WO 1995-US12672 19951002 | | | | |

OTHER SOURCE(S): MARPAT 124:260835
 GI



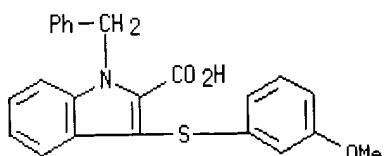
AB Novel indole and indoline nonpeptide antagonists I of endothelin I are described, wherein the dotted line indicates an optional bond; n is 0-4; R1 is Ph, in which the Ph group is substituted by methylenedioxy and further unsubstituted or substituted by, e.g., halo, C1-6 alkyl; R2 is, e.g., H, CO2R, tetrazolyl, R = e.g., H, C1-6 alkyl,; R3 = S(O)pPh, in which p is 0, 1, or 2 and Ph is unsubstituted or substituted by, e.g., halo, NO2, N3; R4 is one to four independent substituents selected from, e.g., hydrogen, alkyl of 1-7 carbon atoms, alkenyl of 2-7 carbon atoms, alkynyl of 2-7 carbon atom, cycloalkyl, Ph; as well as novel intermediates used in their prepn., methods for the prepn. and pharmaceutical compns. of the same, which are useful in treating elevated levels of endothelin, essential renovascular malignant and pulmonary hypertension, cerebral infarction, cerebral **ischemia**, congestive heart failure and subarachnoid hemorrhage. Thus, e.g., phenylsulfonylation of indole-2-carboxylic acid followed by treatment with Cu(II) oxide, 4-iodo-1,2-methylenedioxybenzene, and KOH afforded 1-(benzo[1,3]dioxol-5-yl)-3-phenylsulfanyl-1H-indole-2-carboxylic acid (II). In radioligand binding assays, the following cultured cells were used: rabbit renal artery vascular smooth muscle cells (ERBA-A), Ltk-cells expressing recombinant human ETAR (HERBA-A), and CHO-K1 cells expressing recombinant human ETBR (HERBA-B); II exhibited endothelin receptor binding activity with IC50 = 1.9, 3.2, and 6.5 μ M in the ERBA-A, HERBA-A, and HERBA-B assays, resp.

IT 175339-72-7P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses) (indole-2-carboxylic acids as nonpeptide endothelin antagonists)

RN 175339-72-7 HCAPLUS

CN 1H-Indole-2-carboxylic acid, 3-[(3-methoxyphenyl)thio]-1-(phenylmethyl)-(9CI) (CA INDEX NAME)



=> d his

(FILE 'HOME' ENTERED AT 19:21:10 ON 22 JUN 2004)

FILE 'REGISTRY' ENTERED AT 19:21:16 ON 22 JUN 2004

L1 STRUCTURE UPLOADED
 L2 4 S L1
 L3 579 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 19:22:04 ON 22 JUN 2004

L4 39 S L3/THU
 L5 6 S L4 AND ARTHRITIS?
 L6 1 S L5 AND FAULL, A?/AU
 L7 5 S L5 NOT L6
 L8 33 S L4 NOT L5
 L9 0 S L8 AND GLOMERULAR?
 L10 0 S L8 AND LUNG () FIBROSIS?
 L11 2 S L8 AND RESTENOSIS?
 L12 0 S L11 AND FAULL, A?/AU
 L13 0 S L11 AND KETTLE, J?/AU
 L14 0 S L8 AND ALVEOLITIS?
 L15 3 S L8 AND ASTHMA?
 L16 0 S L15 AND FAULL, A?/AU
 S L1 AND KETTLE, J?/AU

FILE 'REGISTRY' ENTERED AT 19:24:50 ON 22 JUN 2004

L17 4 S L1

FILE 'HCAPLUS' ENTERED AT 19:24:51 ON 22 JUN 2004

L18 4 S L17
 L19 1 S L18 AND KETTLE, J?/AU

FILE 'HCAPLUS' ENTERED AT 19:25:00 ON 22 JUN 2004

L20 3 S L15 NOT L19
 L21 30 S L8 NOT L20
 L22 1 S L21 AND ATHEROSCLEROSIS?
 L23 0 S L22 AND FAULL, A?/AU
 L24 0 S L22 AND KETTLE, J?/AU
 L25 29 S L21 NOT L22
 L26 2 S L25 AND SKIN?
 L27 0 S L26 AND FAULL, A?/AU
 L28 3 S L25 AND KETTLE, J?/AU
 L29 0 S L26 AND KETTLE, J?/AU
 L30 27 S L25 NOT L26
 L31 0 S L30 AND MULTIPLE () SCLEROSIS?
 L32 0 S L30 AND INFLAMM? () BOWEL?
 L33 1 S L30 AND BRAIN () TRAUMA?
 L34 26 S L30 NOT L33
 L35 1 S L34 AND ISCHEMIA?

=> s 134 not 135
 L36 25 L34 NOT L35

=> s 136 and myocardial? () infarction?
 54476 MYOCARDIAL?
 26500 INFARCTION?
 16606 MYOCARDIAL? (W) INFARCTION?
 L37 0 L36 AND MYOCARDIAL? (W) INFARCTION?

=> s 136 and transplant () rejection?
 43773 TRANSPLANT
 7027 TRANSPLANTS
 46697 TRANSPLANT
 (TRANSPLANT OR TRANSPLANTS)
 28759 REJECTION?
 7880 TRANSPLANT (W) REJECTION?
 L38 0 L36 AND TRANSPLANT (W) REJECTION?

=> file caold

| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|--|------------------|---------------|
| FULL ESTIMATED COST | 61.68 | 269.94 |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION |
| CA SUBSCRIBER PRICE | -6.24 | -11.78 |

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FILE COVERS 1907-1966
 FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

This file supports REG1stRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

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FILE 'REGISTRY' ENTERED AT 19:21:16 ON 22 JUN 2004

L1 STRUCTURE uploaded
 L2 4 S L1
 L3 579 S L1 FULL

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 L6 1 S L5 AND FAULL, A?/AU
 L7 5 S L5 NOT L6
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 L9 0 S L8 AND GLOMERULAR?
 L10 0 S L8 AND LUNG () FIBROSIS?
 L11 2 S L8 AND RESTENOSIS?
 L12 0 S L11 AND FAULL, A?/AU
 L13 0 S L11 AND KETTLE, J?/AU
 L14 0 S L8 AND ALVEOLITIS?
 L15 3 S L8 AND ASTHMA?
 L16 0 S L15 AND FAULL, A?/AU
 S L1 AND KETTLE, J?/AU

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L17 4 S L1

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 L24 0 S L22 AND KETTLE, J?/AU
 L25 29 S L21 NOT L22
 L26 2 S L25 AND SKIN?
 L27 0 S L26 AND FAULL, A?/AU
 L28 3 S L25 AND KETTLE, J?/AU
 L29 0 S L26 AND KETTLE, J?/AU
 L30 27 S L25 NOT L26
 L31 0 S L30 AND MULTIPLE () SCLEROSIS?
 L32 0 S L30 AND INFLAMM? () BOWEL?
 L33 1 S L30 AND BRAIN () TRAUMA?
 L34 26 S L30 NOT L33
 L35 1 S L34 AND ISCHEMIA?
 L36 25 S L34 NOT L35
 L37 0 S L36 AND MYOCARDIAL? () INFARCTION?
 L38 0 S L36 AND TRANSPLANT () REJECTION?

FILE 'CAOLD' ENTERED AT 19:29:42 ON 22 JUN 2004

=> s 13 and inflamm?
 7 L3
 1978 INFLAMM?
 L39 0 L3 AND INFLAMM?

=> s 13 and arthrit?
 7 L3
 877 ARTHRIT?
 L40 0 L3 AND ARTHRIT?

=> s 13 and glomerular?
 7 L3
 339 GLOMERULAR?
 L41 0 L3 AND GLOMERULAR?

=> s 13 and lung () fibrosis?
 7 L3
 1393 LUNG
 911 LUNGS
 2281 LUNG
 (LUNG OR LUNGS)
 184 FIBROSIS?
 5 LUNG (W) FIBROSIS?
 L42 0 L3 AND LUNG (W) FIBROSIS?

=> s 13 and restenosis?
 7 L3
 0 RESTENOSIS?
 L43 0 L3 AND RESTENOSIS?

=> s 13 and asthma?
 7 L3
 449 ASTHMA?
 L44 0 L3 AND ASTHMA?

=> s 13 and atherosclerosis?
 7 L3
 1373 ATHEROSCLEROSIS?

L45 0 L3 AND ATHEROSCLEROSIS?

=> s l3 and psoriasis?

7 L3

283 PSORIASIS?

L46 0 L3 AND PSORIASIS?

=> s l3 and skin?

7 L3

7524 SKIN?

L47 0 L3 AND SKIN?

=> s l3 and inflammatory () bowel?

7 L3

570 INFLAMMATORY

74 BOWEL?

0 INFLAMMATORY (W) BOWEL?

L48 0 L3 AND INFLAMMATORY (W) BOWEL?

=> s l3 and multiple () sclerosi?

7 L3

2911 MULTIPLE

10 MULTIPLES

2921 MULTIPLE

(MULTIPLE OR MULTIPLES)

346 SCLEROSI?

171 MULTIPLE (W) SCLEROSI?

L49 0 L3 AND MULTIPLE (W) SCLEROSI?

=> s l3 and brain?

7 L3

7223 BRAIN?

L50 0 L3 AND BRAIN?

=> s l3 and ischemia?

7 L3

216 ISCHEMIA?

L51 0 L3 AND ISCHEMIA?

=> s l3 and infarction?

7 L3

477 INFARCTION?

L52 0 L3 AND INFARCTION?

=> s l3 and transplant () rejection?

7 L3

40 TRANSPLANT

146 TRANSPLANTS

186 TRANSPLANT

(TRANSPLANT OR TRANSPLANTS)

75 REJECTION?

1 TRANSPLANT (W) REJECTION?

L53 0 L3 AND TRANSPLANT (W) REJECTION?

=> s l3 and stroke?

7 L3

85 STROKE?

L54 0 L3 AND STROKE?

=> file reg

| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|--|------------------|---------------|
| FULL ESTIMATED COST | 36.28 | 306.22 |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION |
| CA SUBSCRIBER PRICE | 0.00 | -11.78 |

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STRUCTURE FILE UPDATES: 21 JUN 2004 HIGHEST RN 697224-75-2
 DICTIONARY FILE UPDATES: 21 JUN 2004 HIGHEST RN 697224-75-2

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
<http://www.cas.org/ONLINE/DBSS/registryss.html>

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(FILE 'HOME' ENTERED AT 19:21:10 ON 22 JUN 2004)

FILE 'REGISTRY' ENTERED AT 19:21:16 ON 22 JUN 2004

L1 STRUCTURE uploaded
 L2 4 S L1
 L3 579 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 19:22:04 ON 22 JUN 2004

L4 39 S L3/THU
 L5 6 S L4 AND ARTHRITIS?
 L6 1 S L5 AND FAULL, A?/AU
 L7 5 S L5 NOT L6
 L8 33 S L4 NOT L5
 L9 0 S L8 AND GLOMERULAR?
 L10 0 S L8 AND LUNG () FIBROSIS?
 L11 2 S L8 AND RESTENOSIS?
 L12 0 S L11 AND FAULL, A?/AU
 L13 0 S L11 AND KETTLE, J?/AU
 L14 0 S L8 AND ALVEOLITIS?
 L15 3 S L8 AND ASTHMA?
 L16 0 S L15 AND FAULL, A?/AU
 S L1 AND KETTLE, J?/AU

FILE 'REGISTRY' ENTERED AT 19:24:50 ON 22 JUN 2004

L17 4 S L1

FILE 'HCAPLUS' ENTERED AT 19:24:51 ON 22 JUN 2004

L18 4 S L17
 L19 1 S L18 AND KETTLE, J?/AU

FILE 'HCAPLUS' ENTERED AT 19:25:00 ON 22 JUN 2004

L20 3 S L15 NOT L19
 L21 30 S L8 NOT L20
 L22 1 S L21 AND ATHEROSCLEROSIS?
 L23 0 S L22 AND FAULL, A?/AU
 L24 0 S L22 AND KETTLE, J?/AU
 L25 29 S L21 NOT L22
 L26 2 S L25 AND SKIN?
 L27 0 S L26 AND FAULL, A?/AU
 L28 3 S L25 AND KETTLE, J?/AU
 L29 0 S L26 AND KETTLE, J?/AU
 L30 27 S L25 NOT L26
 L31 0 S L30 AND MULTIPLE () SCLEROSIS?
 L32 0 S L30 AND INFLAMM? () BOWEL?
 L33 1 S L30 AND BRAIN () TRAUMA?
 L34 26 S L30 NOT L33
 L35 1 S L34 AND ISCHEMIA?
 L36 25 S L34 NOT L35
 L37 0 S L36 AND MYOCARDIAL? () INFARCTION?
 L38 0 S L36 AND TRANSPLANT () REJECTION?

FILE 'CAOLD' ENTERED AT 19:29:42 ON 22 JUN 2004

L39 0 S L3 AND INFLAMM?
 L40 0 S L3 AND ARTHRIT?
 L41 0 S L3 AND GLOMERULAR?
 L42 0 S L3 AND LUNG () FIBROSIS?
 L43 0 S L3 AND RESTENOSIS?
 L44 0 S L3 AND ASTHMA?
 L45 0 S L3 AND ATHEROSCLEROSIS?
 L46 0 S L3 AND PSORIASIS?
 L47 0 S L3 AND SKIN?
 L48 0 S L3 AND INFLAMMATORY () BOWEL?
 L49 0 S L3 AND MULTIPLE () SCLEROSIS?
 L50 0 S L3 AND BRAIN?
 L51 0 S L3 AND ISCHEMIA?
 L52 0 S L3 AND INFARCTION?
 L53 0 S L3 AND TRANSPLANT () REJECTION?
 L54 0 S L3 AND STROKE?

FILE 'REGISTRY' ENTERED AT 19:32:13 ON 22 JUN 2004

| => file hcaplus | | SINCE FILE | TOTAL |
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| FULL ESTIMATED COST | | 0.42 | 306.64 |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | | SINCE FILE | TOTAL |
| | | ENTRY | SESSION |
| CA SUBSCRIBER PRICE | | 0.00 | -11.78 |

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FILE COVERS 1907 - 22 Jun 2004 VOL 140 ISS 26
 FILE LAST UPDATED: 21 Jun 2004 (20040621/ED)

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L1 STRUCTURE UPLOADED
 L2 4 S L1
 L3 579 S L1 FULL

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L4 39 S L3/THU
 L5 6 S L4 AND ARTHRITIS?
 L6 1 S L5 AND FAULL, A?/AU
 L7 5 S L5 NOT L6
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 L14 0 S L8 AND ALVEOLITIS?
 L15 3 S L8 AND ASTHMA?
 L16 0 S L15 AND FAULL, A?/AU
 S L1 AND KETTLE, J?/AU

FILE 'REGISTRY' ENTERED AT 19:24:50 ON 22 JUN 2004

L17 4 S L1

FILE 'HCAPLUS' ENTERED AT 19:24:51 ON 22 JUN 2004

L18 4 S L17
 L19 1 S L18 AND KETTLE, J?/AU

FILE 'HCAPLUS' ENTERED AT 19:25:00 ON 22 JUN 2004

L20 3 S L15 NOT L19
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 L27 0 S L26 AND FAULL, A?/AU
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 L29 0 S L26 AND KETTLE, J?/AU
 L30 27 S L25 NOT L26

L31 0 S L30 AND MULTIPLE () SCLEROSIS?
L32 0 S L30 AND INFLAMM? () BOWEL?
L33 1 S L30 AND BRAIN () TRAUMA?
L34 26 S L30 NOT L33
L35 1 S L34 AND ISCHEMIA?
L36 25 S L34 NOT L35
L37 0 S L36 AND MYOCARDIAL? () INFARCTION?
L38 0 S L36 AND TRANSPLANT () REJECTION?

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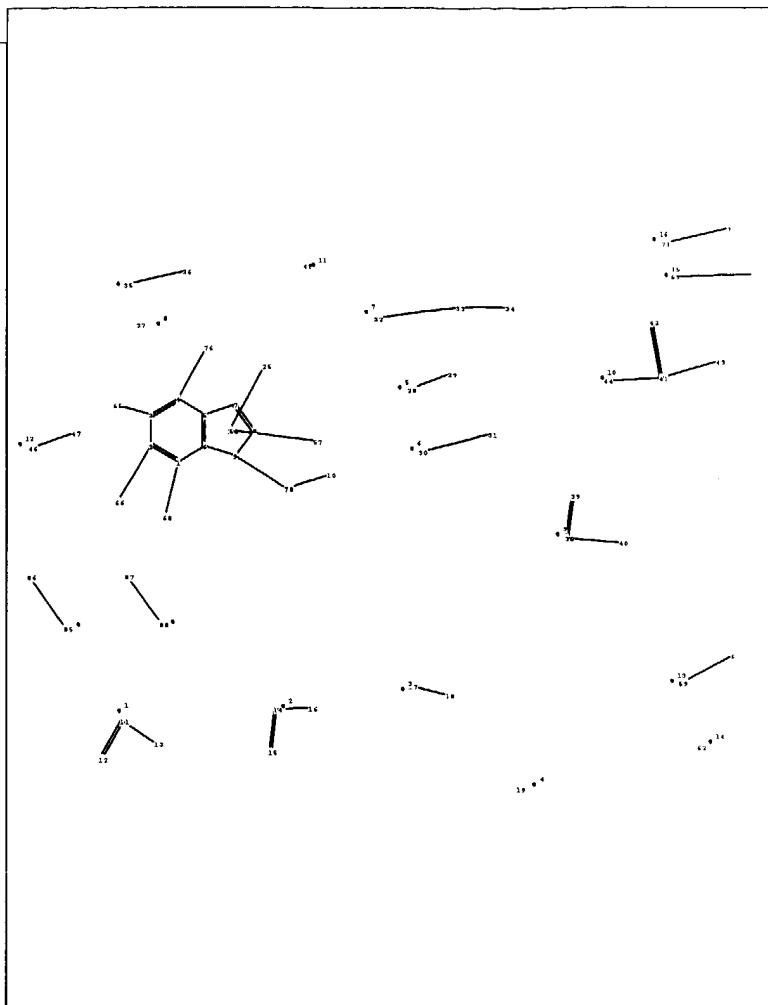
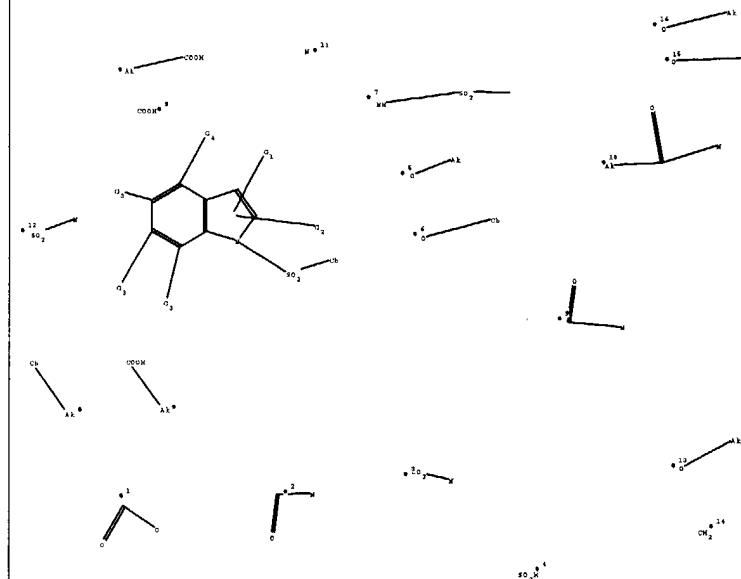
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L43 0 S L3 AND RESTENOSIS?
L44 0 S L3 AND ASTHMA?
L45 0 S L3 AND ATHEROSCLEROSIS?
L46 0 S L3 AND PSORIASIS?
L47 0 S L3 AND SKIN?
L48 0 S L3 AND INFLAMMATORY () BOWEL?
L49 0 S L3 AND MULTIPLE () SCLEROSIS?
L50 0 S L3 AND BRAIN?
L51 0 S L3 AND ISCHEMIA?
L52 0 S L3 AND INFARCTION?
L53 0 S L3 AND TRANSPLANT () REJECTION?
L54 0 S L3 AND STROKE?

FILE 'REGISTRY' ENTERED AT 19:32:13 ON 22 JUN 2004

FILE 'HCAPLUS' ENTERED AT 19:32:22 ON 22 JUN 2004

=> s l36 and stroke?
22846 STROKE?
L55 0 L36 AND STROKE?

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chain nodes :

10 11 12 13 14 15 16 17 18 19 25 28 29 30 31 32 33 35 36 37 38 39
40 41 42 43 44 45 46 47 57 59 60 62 65 66 68 69 70 71 72 76 78 85
86 87 88

ring nodes :

1 2 3 4 5 6 7 8 9

ring/chain nodes :

34

chain bonds :

1-68 2-66 3-65 4-76 9-78 10-78 11-12 11-13 14-15 14-16 14-17 17-18 28-29 30-31
32-33 33-34 35-36 38-39 38-40 41-42 41-43 41-44 46-47 59-60 69-70 71-72 85-86
87-88

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9

exact/norm bonds :

1-68 2-66 3-65 4-76 9-78 11-12 11-13 14-15 14-16 14-17 17-18 28-29 32-33 35-36
38-39 38-40 41-42 41-43 41-44 46-47 59-60 71-72 85-86 87-88

exact bonds :

5-7 6-9 7-8 8-9 10-78 30-31 33-34 69-70

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

containing 1 :

G1:[*1],[*2],[*3],[*4]

G2:[*5],[*6],[*7],[*8],[*9],[*10],[*11],[*12]

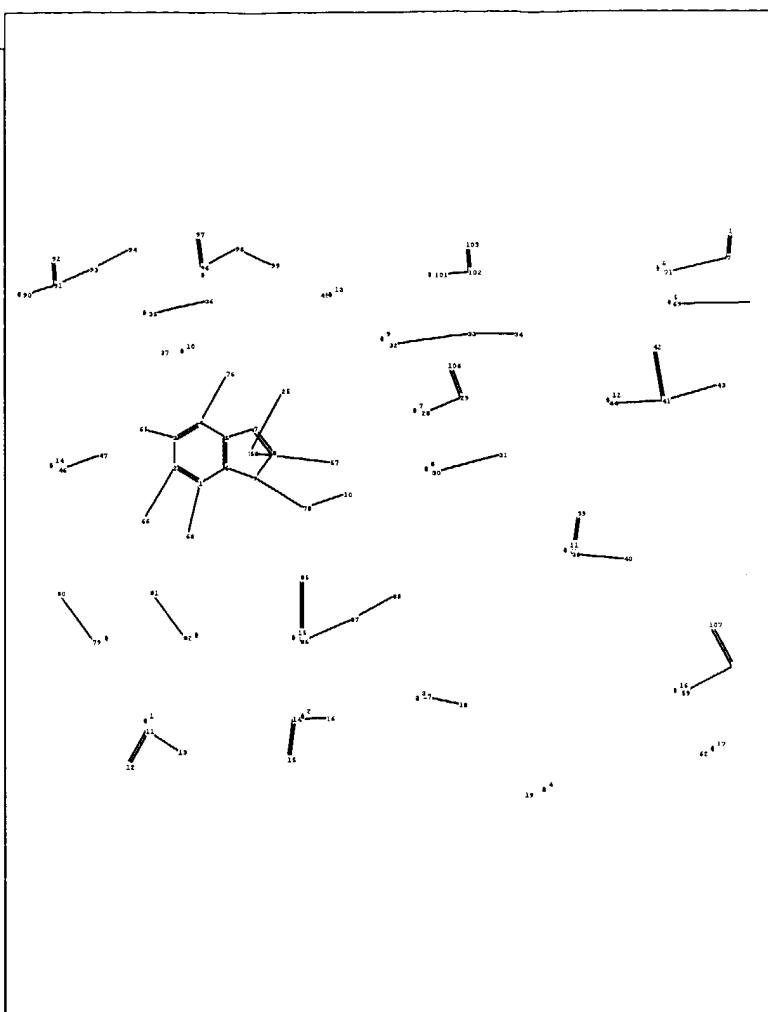
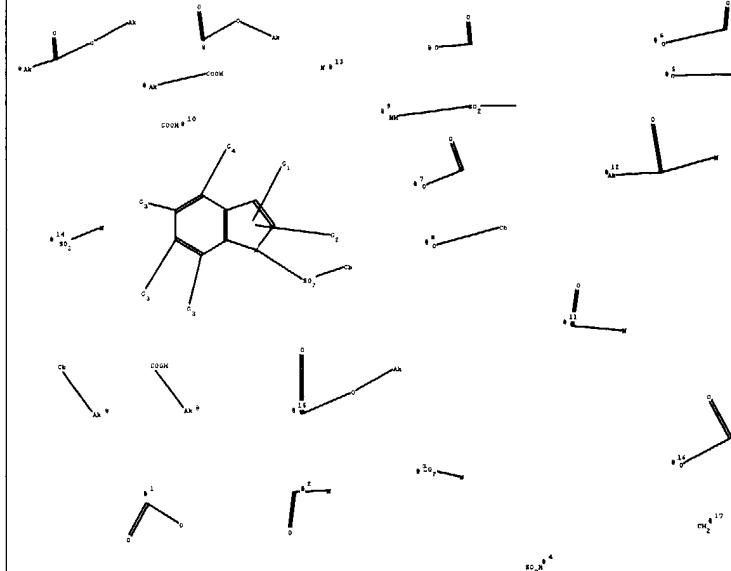
G3:H,OH,X,[*13],[*14]

G4:[*1],[*2],[*15],[*16]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:CLASS
12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 25:CLASS
26:CLASS 28:CLASS 29:CLASS 30:CLASS 31:Atom 32:CLASS 33:CLASS 34:CLASS 35:CLASS
36:CLASS 37:CLASS 38:CLASS 39:CLASS 40:CLASS 41:CLASS 42:CLASS 43:CLASS 44:CLASS
45:CLASS 46:CLASS 47:CLASS 57:CLASS 58:CLASS 59:CLASS 60:CLASS 62:CLASS 65:CLASS
66:CLASS 68:CLASS 69:CLASS 70:Atom 71:CLASS 72:CLASS 76:CLASS 78:CLASS 85:CLASS
86:Atom 87:CLASS 88:CLASS

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chain nodes :

10 11 12 13 14 15 16 17 18 19 25 28 29 30 31 32 33 35 36 38 39 40 41 42 43 44 45 46 47 57 59 60 62 65 66 68 69 70 71 72 76 78 79 80 81 82 85 86 87 88 90 91 92 93 94 96 97 98 99 101 102 103 105 106 107

ring nodes :

1 2 3 4 5 6 7 8 9

ring/chain nodes :

34

chain bonds :

1-68 2-66 3-65 4-76 9-78 10-78 11-12 11-13 14-15 14-16 17-18 28-29 29-106
30-31 32-33 33-34 35-36 38-39 38-40 41-42 41-43 41-44 46-47 59-60 60-107
69-70 71-72 72-105 79-80 81-82 85-86 86-87 87-88 90-91 91-92 91-93 93-94
96-97 96-98 98-99 101-102 102-103

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9

exact/norm bonds :

1-68 2-66 3-65 4-76 9-78 11-12 11-13 14-15 14-16 17-18 28-29 29-106 32-33
35-36 38-39 38-40 41-42 41-43 41-44 46-47 59-60 60-107 71-72 72-105 79-80
81-82 85-86 86-87 87-88 90-91 91-92 91-93 93-94 96-97 96-98 98-99 101-102
102-103

exact bonds :

5-7 6-9 7-8 8-9 10-78 30-31 33-34 69-70

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

containing 1 :

G1:[*1],[*2],[*3],[*4],[*5],[*6]

G2:[*7],[*8],[*9],[*10],[*11],[*12],[*13],[*14],[*15]

G3:H,OH,X,[*16],[*17]

G4:[*1],[*2],[*5],[*6]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:CLASS
12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 25:CLASS
26:CLASS 28:CLASS 29:CLASS 30:CLASS 31:Atom 32:CLASS 33:CLASS 34:CLASS 35:CLASS
36:CLASS 37:CLASS 38:CLASS 39:CLASS 40:CLASS 41:CLASS 42:CLASS 43:CLASS 44:CLASS
45:CLASS 46:CLASS 47:CLASS 57:CLASS 58:CLASS 59:CLASS 60:CLASS 62:CLASS 65:CLASS
66:CLASS 68:CLASS 69:CLASS 70:Atom 71:CLASS 72:CLASS 76:CLASS 78:CLASS 79:CLASS
80:Atom 81:CLASS 82:CLASS 85:CLASS 86:CLASS 87:CLASS 88:CLASS 90:CLASS 91:CLASS
92:CLASS 93:CLASS 94:CLASS 96:CLASS 97:CLASS 98:CLASS 99:CLASS 101:CLASS
102:CLASS 103:CLASS 105:CLASS 106:CLASS 107:CLASS

| | | |
|---------------------|--|--|
| <u>NEWS</u> 1 | Web Page URLs for STN Seminar Schedule - N. America | |
| <u>NEWS</u> 2 | "Ask CAS" for self-help around the clock | |
| <u>NEWS</u> 3 | May 10 | PROUSDDR now available on STN |
| <u>NEWS</u> 4 | May 19 | PROUSDDR: One FREE connect hour, per account, in both May and June 2004 |
| <u>NEWS</u> 5 | May 12 | EXTEND option available in structure searching |
| <u>NEWS</u> 6 | May 12 | Polymer links for the POLYLINK command completed in REGISTRY |
| <u>NEWS</u> 7 | May 17 | FRFULL now available on STN |
| <u>NEWS</u> 8 | May 27 | New UPM (Update Code Maximum) field for more efficient patent SDIs in CAplus |
| <u>NEWS</u> 9 | May 27 | CAplus super roles and document types searchable in REGISTRY |
| <u>NEWS</u> 10 | May 27 | Explore APOLLIT with free connect time in June 2004 |
| <u>NEWS</u> 11 | Jun 22 | STN Patent Forums to be held July 19-22, 2004 |
| <u>NEWS EXPRESS</u> | MARCH 31 CURRENT WINDOWS VERSION IS V7.00A, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 26 APRIL 2004 | |
| <u>NEWS HOURS</u> | STN Operating Hours Plus Help Desk Availability | |
| <u>NEWS INTER</u> | General Internet Information | |
| <u>NEWS LOGIN</u> | Welcome Banner and News Items | |
| <u>NEWS PHONE</u> | Direct Dial and Telecommunication Network Access to STN | |
| <u>NEWS WWW</u> | CAS World Wide Web Site (general information) | |

Enter NEWS followed by the item number or name to see news on that specific topic.

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FILE 'HOME' ENTERED AT 20:15:05 ON 22 JUN 2004

=> file reg
COST IN U.S. DOLLARS
SINCE FILE ENTRY TOTAL
SESSION
FULL ESTIMATED COST 0.21 0.21

FILE 'REGISTRY' ENTERED AT 20:15:12 ON 22 JUN 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2004 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 21 JUN 2004 HIGHEST RN 697224-75-2
DICTIONARY FILE UPDATES: 21 JUN 2004 HIGHEST RN 697224-75-2

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
<http://www.cas.org/ONLINE/DBSS/registrys.html>

```
=>
L1      STRUCTURE UPLOADED

=> d 11
L1 HAS NO ANSWERS
L1      STR

=> s 11
SAMPLE SEARCH INITIATED 20:17:09 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -      2 TO ITERATE

100.0% PROCESSED      2 ITERATIONS          0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:      2 TO      124
PROJECTED ANSWERS:          0 TO      0
```

```
L2      0 SEA SSS SAM L1

=> s 11 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 20:17:14 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -      5 TO ITERATE

100.0% PROCESSED      5 ITERATIONS          0 ANSWERS
SEARCH TIME: 00.00.01
```

```
L3      0 SEA SSS FUL L1

=>
L4      STRUCTURE UPLOADED

=> d 14
L4 HAS NO ANSWERS
L4      STR

=> s 14
SAMPLE SEARCH INITIATED 20:27:04 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -      0 TO ITERATE
```

```
100.0% PROCESSED      0 ITERATIONS          0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:      0 TO      0
PROJECTED ANSWERS:          0 TO      0
```

```
L5      0 SEA SSS SAM L4

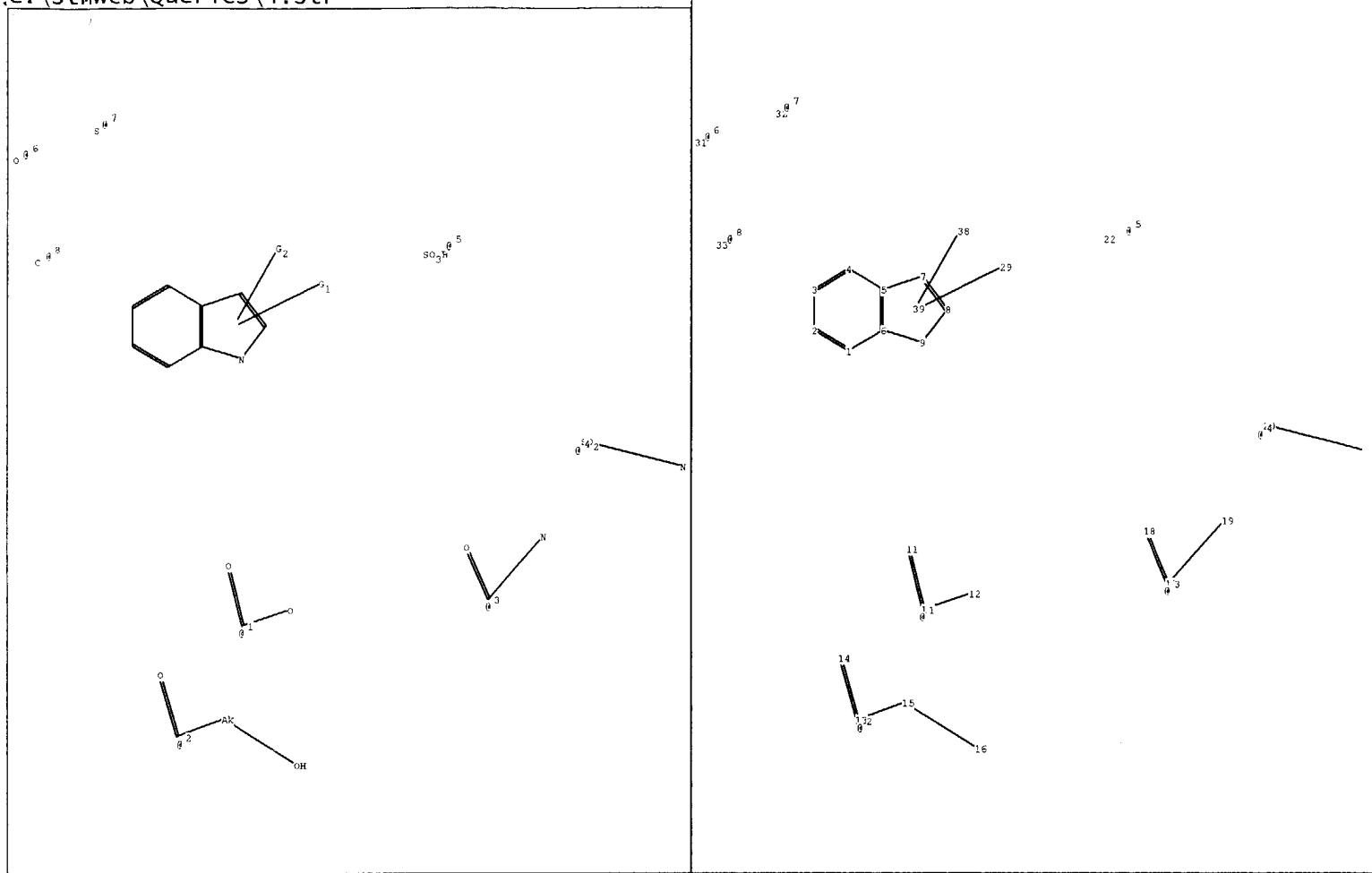
=> s 14 full
```

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 20:27:08 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 1 TO ITERATE

100.0% PROCESSED 1 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

L6 0 SEA SSS FUL L4

=>



chain nodes :

10 11 12 13 14 15 16 17 18 19 20 21 22 29 31 32 33 38

ring nodes :

1 2 3 4 5 6 7 8 9

chain bonds :

10-12 10-11 13-14 13-15 15-16 17-18 17-19 20-21

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9

exact/norm bonds :

6-9 8-9 10-12 10-11 13-14 13-15 15-16 17-18 17-19 20-21

exact bonds :

5-7 7-8

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

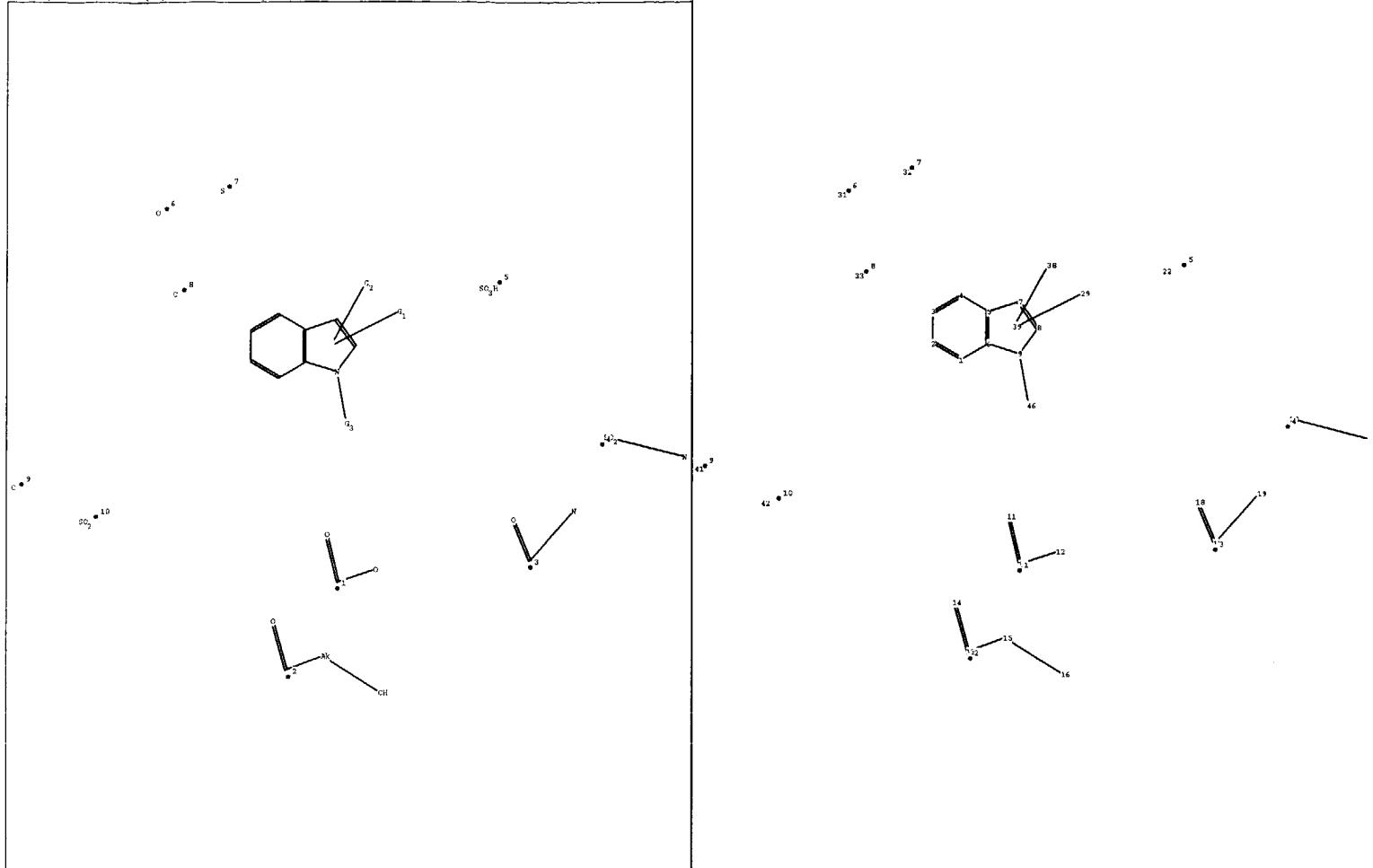
containing 1 :

G1:CN,[*1],[*2],[*3],[*4],[*5]

G2:[*6],[*7],[*8]

Match level :

| | | | | | | | | | |
|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|
| 1:Atom | 2:Atom | 3:Atom | 4:Atom | 5:Atom | 6:Atom | 7:Atom | 8:Atom | 9:Atom | 10:CLASS |
| 11:CLASS | 12:CLASS | 13:CLASS | 14:CLASS | 15:CLASS | 16:CLASS | 17:CLASS | 18:CLASS | 19:CLASS | |
| 20:CLASS | 21:CLASS | 22:CLASS | 29:CLASS | 30:CLASS | 31:CLASS | 32:CLASS | 33:CLASS | 38:CLASS | |
| 39:CLASS | | | | | | | | | |



chain nodes :

10 11 12 13 14 15 16 17 18 19 20 21 22 29 31 32 33 38 41 42 46

ring nodes :

1 2 3 4 5 6 7 8 9

chain bonds :

9-46 10-12 10-11 13-14 13-15 15-16 17-18 17-19 20-21

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9

exact/norm bonds :

6-9 8-9 9-46 10-12 10-11 13-14 13-15 15-16 17-18 17-19 20-21

exact bonds :

5-7 7-8

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

containing 1 :

G1:CN,[*1],[*2],[*3],[*4],[*5]

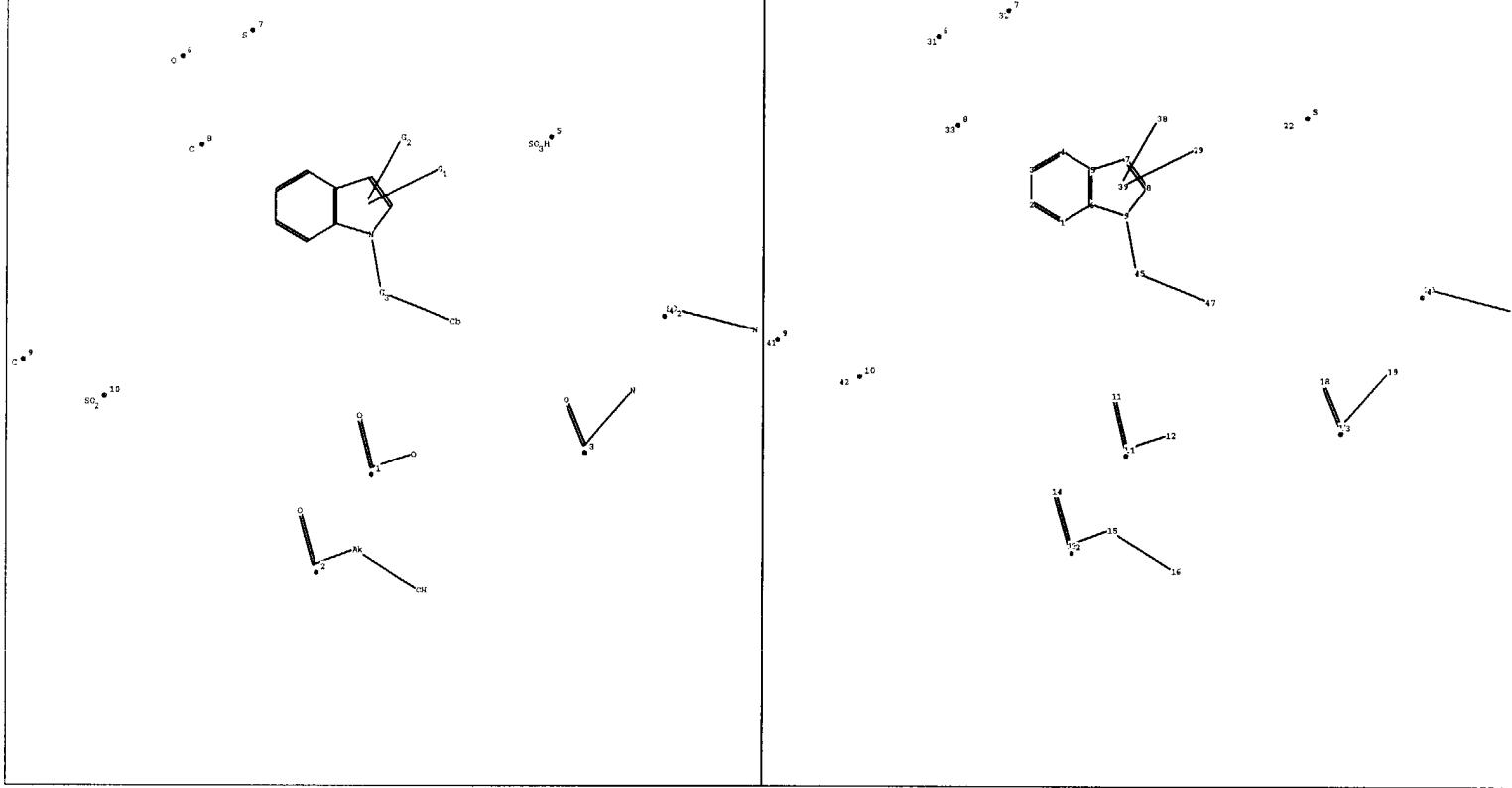
G2:[*6],[*7],[*8]

G3:H,[*9],[*10]

Match level :

| | | | | | | | | | |
|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|
| 1:Atom | 2:Atom | 3:Atom | 4:Atom | 5:Atom | 6:Atom | 7:Atom | 8:Atom | 9:Atom | 10:CLASS |
| 11:CLASS | 12:CLASS | 13:CLASS | 14:CLASS | 15:CLASS | 16:CLASS | 17:CLASS | 18:CLASS | 19:CLASS | |
| 20:CLASS | 21:CLASS | 22:CLASS | 29:CLASS | 30:CLASS | 31:CLASS | 32:CLASS | 33:CLASS | 38:CLASS | |
| 39:CLASS | 41:CLASS | 42:CLASS | 46:CLASS | | | | | | |

C:\stnweb\Queries\3.str



chain nodes :

10 11 12 13 14 15 16 17 18 19 20 21 22 29 31 32 33 38 41 42 45 47

ring nodes :

1 2 3 4 5 6 7 8 9

chain bonds :

9-45 10-12 10-11 13-14 13-15 15-16 17-18 17-19 20-21 45-47

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9

exact/norm bonds :

6-9 8-9 9-45 10-12 10-11 13-14 13-15 15-16 17-18 17-19 20-21 45-47

exact bonds :

5-7 7-8

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

containing 1 :

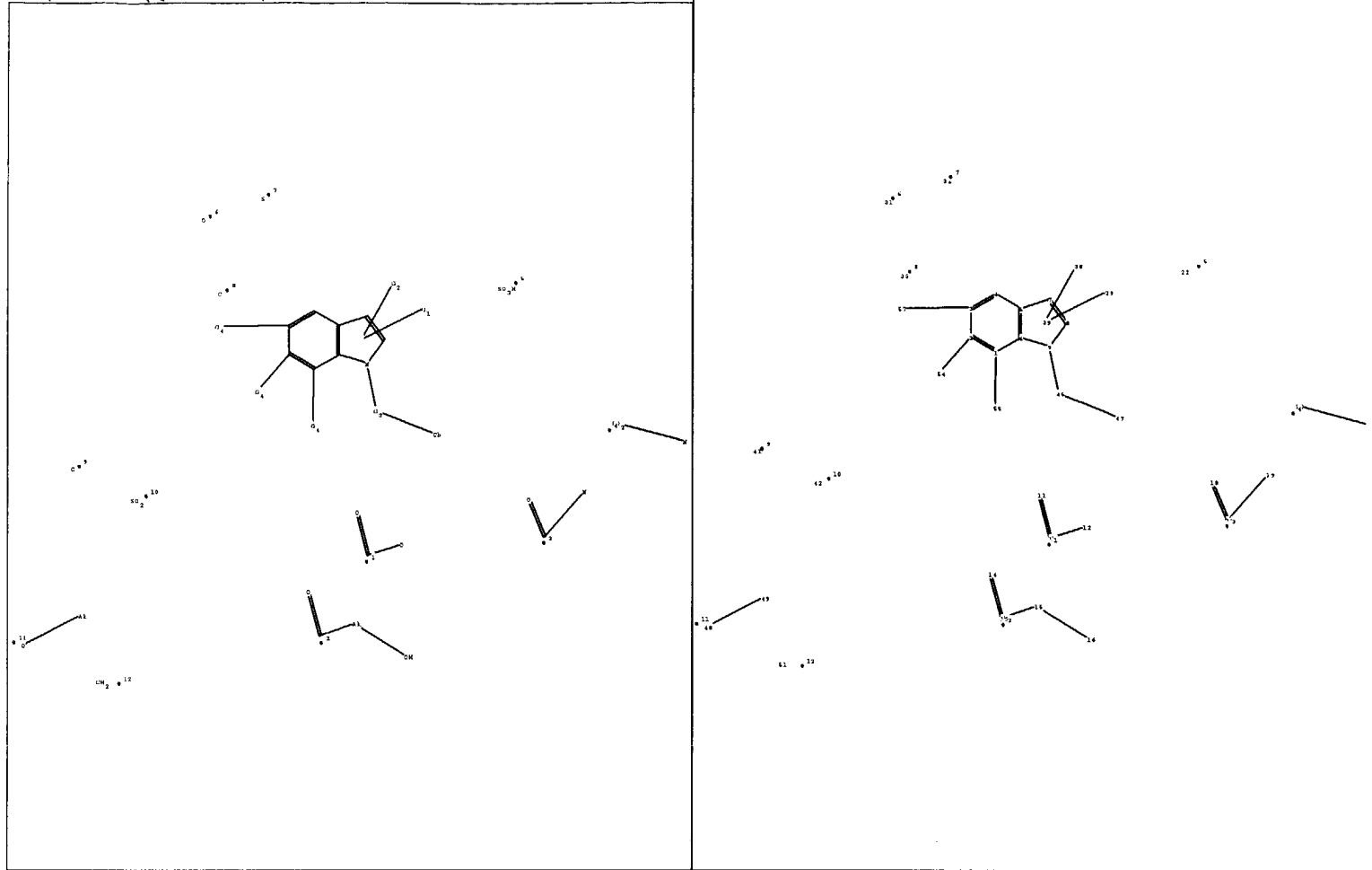
G1:CN,[*1],[*2],[*3],[*4],[*5]

G2:[*6],[*7],[*8]

G3:[*9],[*10]

Match level :

| | | | | | | | | | |
|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|
| 1:Atom | 2:Atom | 3:Atom | 4:Atom | 5:Atom | 6:Atom | 7:Atom | 8:Atom | 9:Atom | 10:CLASS |
| 11:CLASS | 12:CLASS | 13:CLASS | 14:CLASS | 15:CLASS | 16:CLASS | 17:CLASS | 18:CLASS | 19:CLASS | |
| 20:CLASS | 21:CLASS | 22:CLASS | 29:CLASS | 30:CLASS | 31:CLASS | 32:CLASS | 33:CLASS | 38:CLASS | |
| 39:CLASS | 41:CLASS | 42:CLASS | 45:CLASS | 47:Atom | | | | | |



```

chain nodes :
 10 11 12 13 14 15 16 17 18 19 20 21 22 29 31 32 33 38 41 42 45 47
 48 49 51 54 55 57
ring nodes :
 1 2 3 4 5 6 7 8 9
chain bonds :
 1-55 2-54 3-57 9-45 10-12 10-11 13-14 13-15 15-16 17-18 17-19 20-21 45-47
 48-49
ring bonds :
 1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9
exact/norm bonds :
 1-55 2-54 3-57 6-9 8-9 9-45 10-12 10-11 13-14 13-15 15-16 17-18 17-19 20-21
 45-47 48-49
exact bonds :
 5-7 7-8
normalized bonds :
 1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
 containing 1 :

```

G1:CN, [*1], [*2], [*3], [*4], [*5]

G2: [*6], [*7], [*8]

G3: [*9], [*10]

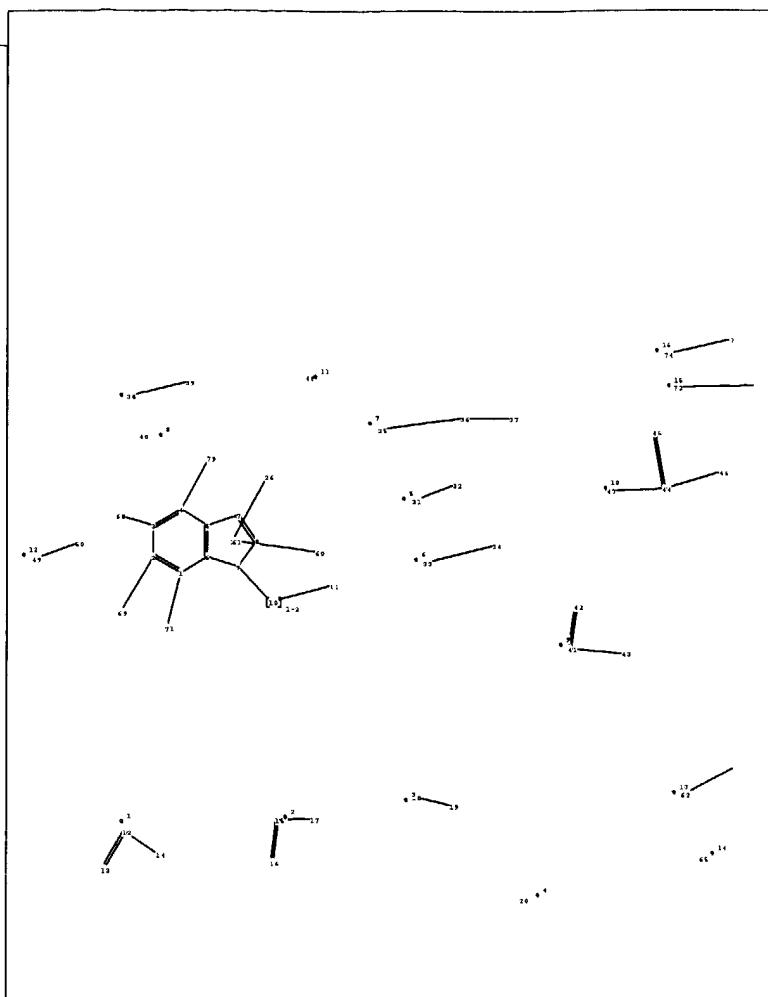
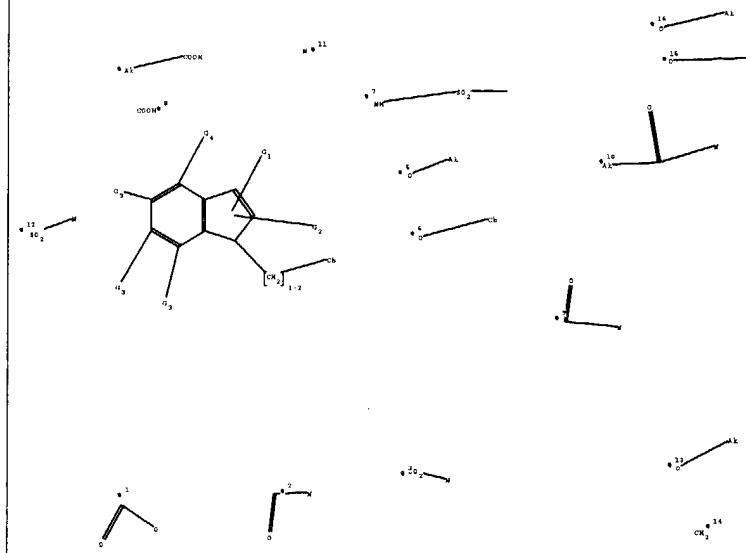
G4:X,H,[*11],[*12]

Match level :

1. ALUM 2
11: CLASS

11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS
20:CLASS 21:CLASS 22:CLASS 29:CLASS 30:CLASS 31:CLASS 32:CLASS 33:CLASS 38:CLASS
39:CLASS 41:CLASS 42:CLASS 45:CLASS 47:Atom 48:CLASS 49:CLASS 51:CLASS 54:CLASS
55:CLASS

c:\stnweb\Queries\4.str



chain nodes :

10 11 12 13 14 15 16 17 18 19 20 26 31 32 33 34 35 36 38 39 40 41
42 43 44 45 46 47 48 49 50 60 62 63 65 68 69 71 72 73 74 75 79

ring nodes :

1 2 3 4 5 6 7 8 9

ring/chain nodes :

37

chain bonds :

1-71 2-69 3-68 4-79 9-10 10-11 12-13 12-14 15-16 15-17 18-19 31-32 33-34
35-36 36-37 38-39 41-42 41-43 44-45 44-46 44-47 49-50 62-63 72-73 74-75

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9

exact/norm bonds :

1-71 2-69 3-68 4-79 12-13 12-14 15-16 15-17 18-19 31-32 35-36 38-39 41-42
41-43 44-45 44-46 44-47 49-50 62-63 74-75

exact bonds :

5-7 6-9 7-8 8-9 9-10 10-11 33-34 36-37 72-73

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

containing 1 :

G1:[*1],[*2],[*3],[*4]

G2:[*5],[*6],[*7],[*8],[*9],[*10],[*11],[*12]

G3:H,OH,X,[*13],[*14]

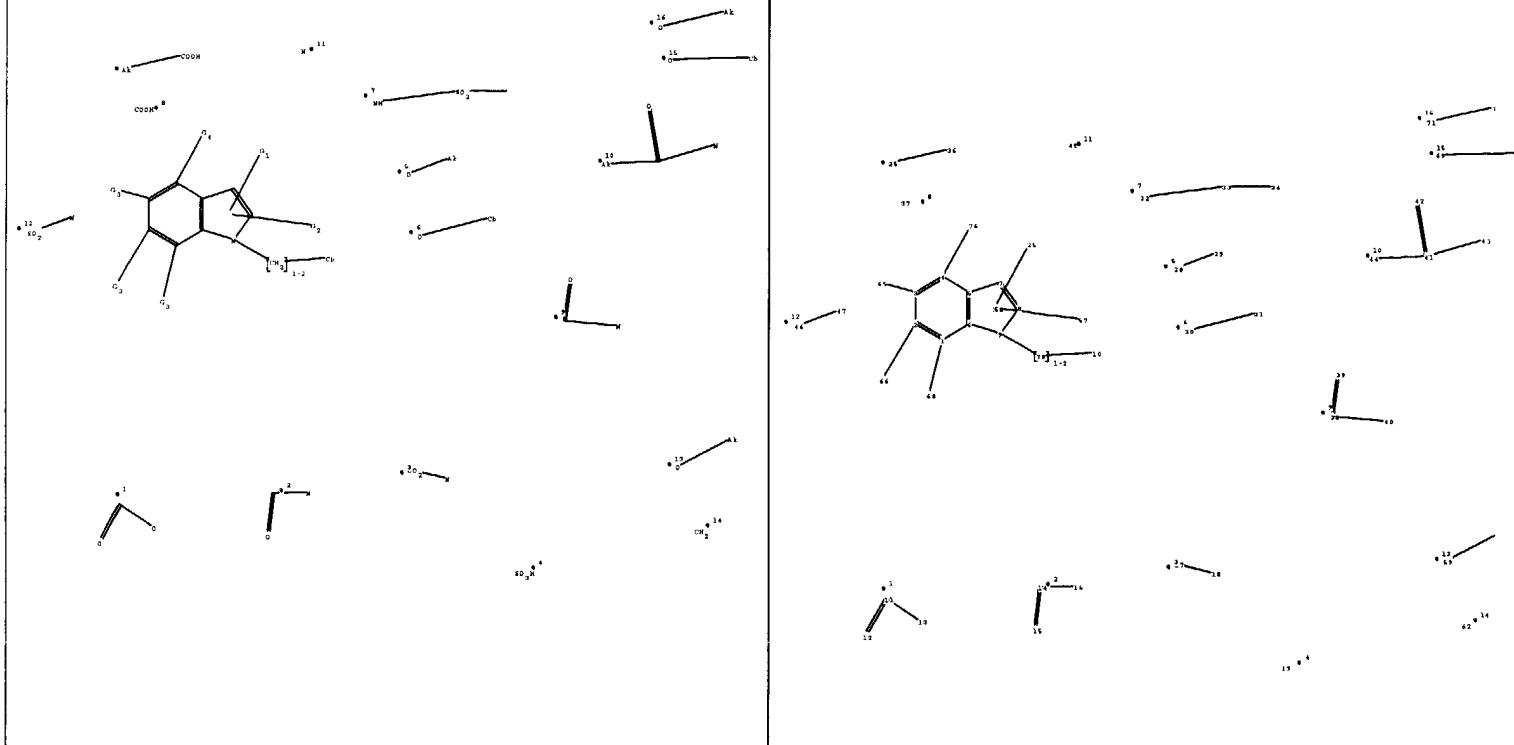
G4:[*15],[*16]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS 11:Atom
12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS
26:CLASS

27:CLASS 31:CLASS 32:CLASS 33:CLASS 34:Atom 35:CLASS 36:CLASS 37:CLASS
38:CLASS 39:CLASS 40:CLASS 41:CLASS 42:CLASS 43:CLASS 44:CLASS 45:CLASS 46:CLASS
47:CLASS 48:CLASS 49:CLASS 50:CLASS 60:CLASS 61:CLASS 62:CLASS 63:CLASS 65:CLASS
68:CLASS 69:CLASS 71:CLASS 72:CLASS 73:Atom 74:CLASS 75:CLASS 79:CLASS

C:\strweb\Queries\4.str



chain nodes :

10 11 12 13 14 15 16 17 18 19 25 28 29 30 31 32 33 35 36 37 38 39
40 41 42 43 44 45 46 47 57 59 60 62 65 66 68 69 70 71 72 76 78

ring nodes :

1 2 3 4 5 6 7 8 9

ring/chain nodes :

34

chain bonds :

1-68 2-66 3-65 4-76 9-78 10-78 11-12 11-13 14-15 14-16 14-17 17-18 28-29 30-31
32-33 33-34 35-36 38-39 38-40 41-42 41-43 41-44 46-47 59-60 69-70 71-72

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9

exact/norm bonds :

1-68 2-66 3-65 4-76 11-12 11-13 14-15 14-16 14-17 17-18 28-29 32-33 35-36 38-39
38-40 41-42 41-43 41-44 46-47 59-60 71-72

exact bonds :

5-7 6-9 7-8 8-9 9-78 10-78 30-31 33-34 69-70

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

containing 1 :

G1:[*1],[*2],[*3],[*4]

G2:[*5],[*6],[*7],[*8],[*9],[*10],[*11],[*12]

G3:H,OH,X,[*13],[*14]

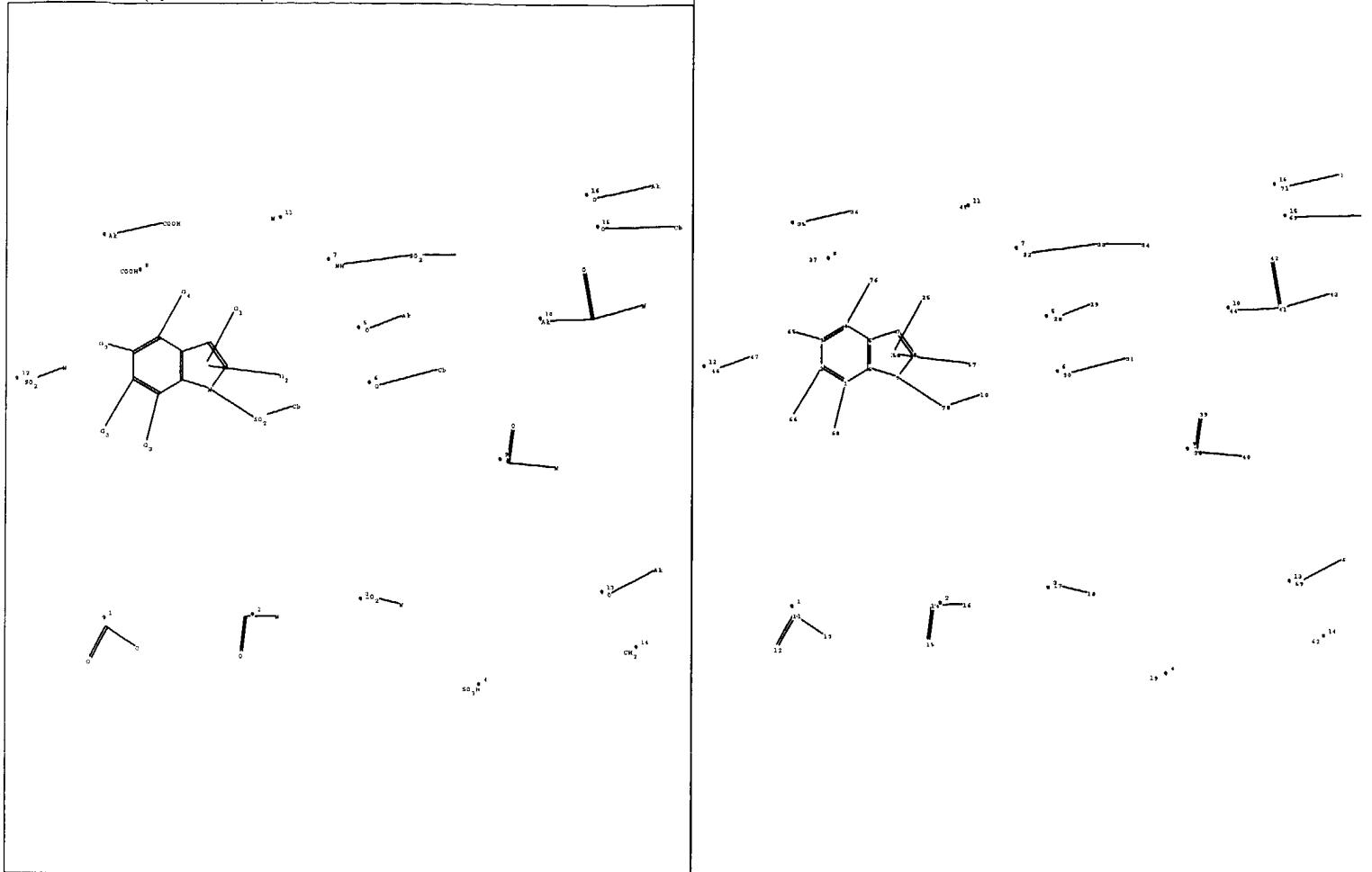
G4:[*15],[*16]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:CLASS
12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 25:CLASS
26:CLASS

28:CLASS 29:CLASS 30:CLASS 31:Atom 32:CLASS 33:CLASS 34:CLASS 35:CLASS
36:CLASS 37:CLASS 38:CLASS 39:CLASS 40:CLASS 41:CLASS 42:CLASS 43:CLASS 44:CLASS
45:CLASS 46:CLASS 47:CLASS 57:CLASS 58:CLASS 59:CLASS 60:CLASS 62:CLASS 65:CLASS
66:CLASS 68:CLASS 69:CLASS 70:Atom 71:CLASS 72:CLASS 76:CLASS 78:CLASS

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28:CLASS 29:CLASS 30:CLASS 31:Atom 32:CLASS 33:CLASS 34:CLASS 35:CLASS
36:CLASS 37:CLASS 38:CLASS 39:CLASS 40:CLASS 41:CLASS 42:CLASS 43:CLASS 44:CLASS
45:CLASS 46:CLASS 47:CLASS 57:CLASS 58:CLASS 59:CLASS 60:CLASS 62:CLASS 65:CLASS
66:CLASS 68:CLASS 69:CLASS 70:Atom 71:CLASS 72:CLASS 76:CLASS 78:CLASS

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:

<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>
L1 STRUCTURE UPLOADED

=> d 11
L1 HAS NO ANSWERS
L1 STR

=> s 11
SAMPLE SEARCH INITIATED 18:53:34 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 18 TO ITERATE

100.0% PROCESSED 18 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
 BATCH **COMPLETE**
PROJECTED ITERATIONS: 106 TO 614
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s 11 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 18:53:39 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 455 TO ITERATE

100.0% PROCESSED 455 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

L3 0 SEA SSS FUL L1

=>
L4 STRUCTURE UPLOADED

=> d 14
L4 HAS NO ANSWERS
L4 STR

=> s 14
SAMPLE SEARCH INITIATED 18:55:11 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 23 TO ITERATE

100.0% PROCESSED 23 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**
 PROJECTED ITERATIONS: 173 TO 747
 PROJECTED ANSWERS: 0 TO 0

L5 0 SEA SSS SAM L4

=> s 14 full
 THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS
 DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
 FULL SEARCH INITIATED 18:55:16 FILE 'REGISTRY'
 FULL SCREEN SEARCH COMPLETED - 527 TO ITERATE

100.0% PROCESSED 527 ITERATIONS 0 ANSWERS
 SEARCH TIME: 00.00.01

L6 0 SEA SSS FUL L4

=>
 L7 STRUCTURE UPLOADED

=> 17
 L7 IS NOT A RECOGNIZED COMMAND
 The previous command name entered was not recognized by the system.
 For a list of commands available to you in the current file, enter
"HELP COMMANDS" at an arrow prompt (=>).

=> d 17
 L7 HAS NO ANSWERS
 L7 STR

=> s 17
 SAMPLE SEARCH INITIATED 18:56:19 FILE 'REGISTRY'
 SAMPLE SCREEN SEARCH COMPLETED - 0 TO ITERATE

100.0% PROCESSED 0 ITERATIONS 0 ANSWERS
 SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
 BATCH **COMPLETE**
 PROJECTED ITERATIONS: 0 TO 0
 PROJECTED ANSWERS: 0 TO 0

L8 0 SEA SSS SAM L7

=> s 17 full
 THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS
 DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
 FULL SEARCH INITIATED 18:56:26 FILE 'REGISTRY'
 FULL SCREEN SEARCH COMPLETED - 10 TO ITERATE

100.0% PROCESSED 10 ITERATIONS 0 ANSWERS
 SEARCH TIME: 00.00.01

L9 0 SEA SSS FUL L7

=>